A Hydrogen Containment Process for Nuclear Thermal Engine Ground testing

Ten-See Wang, Eric Stewart, and Francisco Canabal

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Introduction

- A safe, robust and affordable hydrogen (H2) removal process is necessary to enable the testing required for nuclear thermal propulsion (NTP) engine development.
- A system-level concept had been proposed by burning H2 and cooling the exhaust with direct water spray. However, it omits first-order physics, creating safety and cost issues concerning the H2 containment and the large amounts of non-recyclable water.
- A new process is proposed that meets design objectives. The process will be demonstrated with high fidelity computational design and analysis tools with pertinent physical models.

Objective

- The objective of this study is to propose a new total hydrogen containment process to enable the testing required for NTP engine development. This H_2 removal process comprises of two unit operations: an oxygen-rich burner and a shell-and-tube type of heat exchanger. This new process is demonstrated by simulation of the steady-state operation of the engine firing at nominal conditions.

UNIC Multidisciplinary Computational Fluid Dynamics Methodology

- Unstructured-grid, pressure-based, turbulent, finite-rate reacting flow formulation
- Real Fluid Model for multiphase flows

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho\left(u_j - u_{jg}\right)\right] = 0 \tag{1}$$

$$\frac{\partial \rho \alpha_i}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho\left(u_j - u_{jg}\right)\alpha_i\right] = \frac{\partial}{\partial x_j}\left[\left(\rho D + \frac{\mu_t}{\sigma_\alpha}\right)\frac{\partial \alpha_i}{\partial x_j}\right] + \omega_i \tag{2}$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho\left(u_j - u_{jg}\right)u_i\right] = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \tag{3}$$

$$\frac{\partial \rho H}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho\left(u_j - u_{jg}\right)H\right] = \frac{\partial p}{\partial t} + Q_r + \frac{\partial}{\partial x_j}\left(\left(\frac{K}{C_p} + \frac{\mu_t}{\sigma_H}\right)\nabla H\right) + \frac{\partial}{\partial x_j}\left(\left(\left(\mu + \mu_t\right) - \left(\frac{K}{C_p} + \frac{\mu_t}{\sigma_H}\right)\right)\nabla\left(V^2/2\right)\right) \tag{4}$$

$$+ \frac{\partial}{\partial x_j}\left(\left(\frac{K}{C_p} + \frac{\mu_t}{\sigma_H}\right)\left(u_k\frac{\partial u_j}{\partial x_k} - \frac{2}{3}u_j\frac{\partial u_k}{\partial x_k}\right)\right)$$

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho\left(u_j - u_{jg}\right)k\right] = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + \rho\left(\Pi - \varepsilon\right) \tag{5}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_j}\left[\rho\left(u_j - u_{jg}\right)\varepsilon\right] = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + \rho\frac{\varepsilon}{k}\left(C_1\Pi - C_2\varepsilon + C_3\Pi^2/\varepsilon\right) \tag{6}$$

Heat Exchanger Sizing Methodology

$$\frac{d\rho}{\rho} + \frac{du}{u} = 0$$

$$dp + \frac{4\tau_w dx}{D} + \rho u du = 0$$

$$\dot{Q} = \dot{m}\left(i_2 + \frac{1}{2}u_2^2 - i_1 - \frac{1}{2}u_1^2\right)$$

The power transfer is calculated with Newton's law of cooling as given by:

$$\dot{Q} = hA(T_w - T_m)$$

The local Nusselt number, used to determine the heat transfer coefficient, is obtained from the Gnielinski equation:

$$Nu_D = \frac{(f/8)(Re_D - 1000)Pr}{1 + 12.7(f/8)^{1/2}(Pr^{2/3} - 1)}$$

Where the Moody friction factor for a smooth wall is given as a function of Reynolds number by the Petukhov equation:

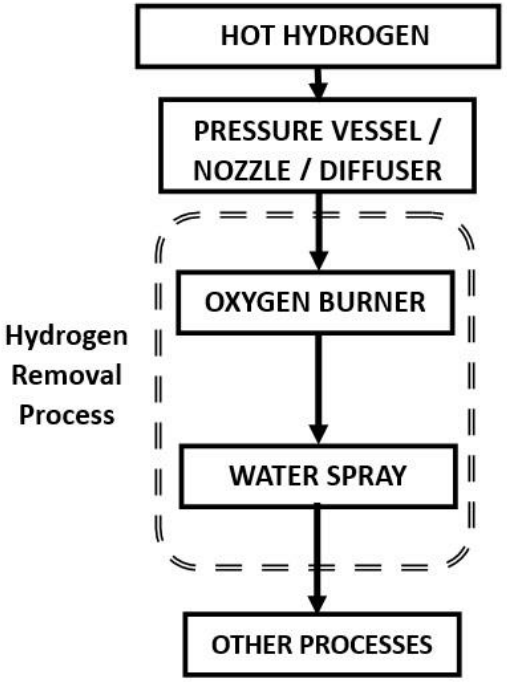
$$f = (0.790\ln(Re_D) - 1.64)^{-2}$$

Which is also used to define the wall shear stress as:

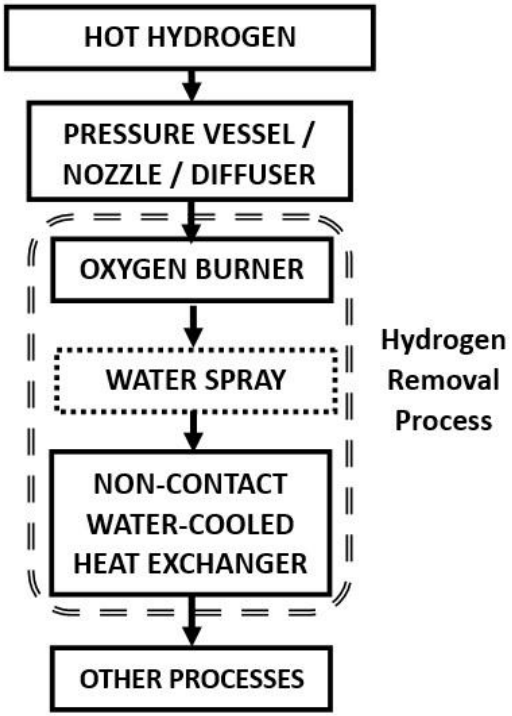
$$\tau_w = f\left(\frac{\rho u_m^2}{8}\right)$$

The software Cequel™ (Chemical Equilibrium in Excel), provides the remaining required equation of state functionality and relations for the transport and thermodynamic properties of the combustion gases, which are allowed to dissociate and recombined through the tube assuming equilibrium throughout.

Total Hydrogen Containment Process



Current process based on system-level model.



The proposed new hydrogen removal process based on the CFD model.

Conceptual Design

Conceptual Design Goals

- Oxygen-Rich Burner design goal: 99% reduction of hydrogen
  - Straight-cylinder burner size
  - State of inlet oxygen
  - O/F ratio
- Heat exchanger design goal: 1% reduction of hydrogen
  - Shell-and-tube tubular heat exchanger
  - Cooling tube size
  - Number of cooling tubes
  - Layout of cooling tubes
- Hydrogen removal process goal: computed flammability < LFL

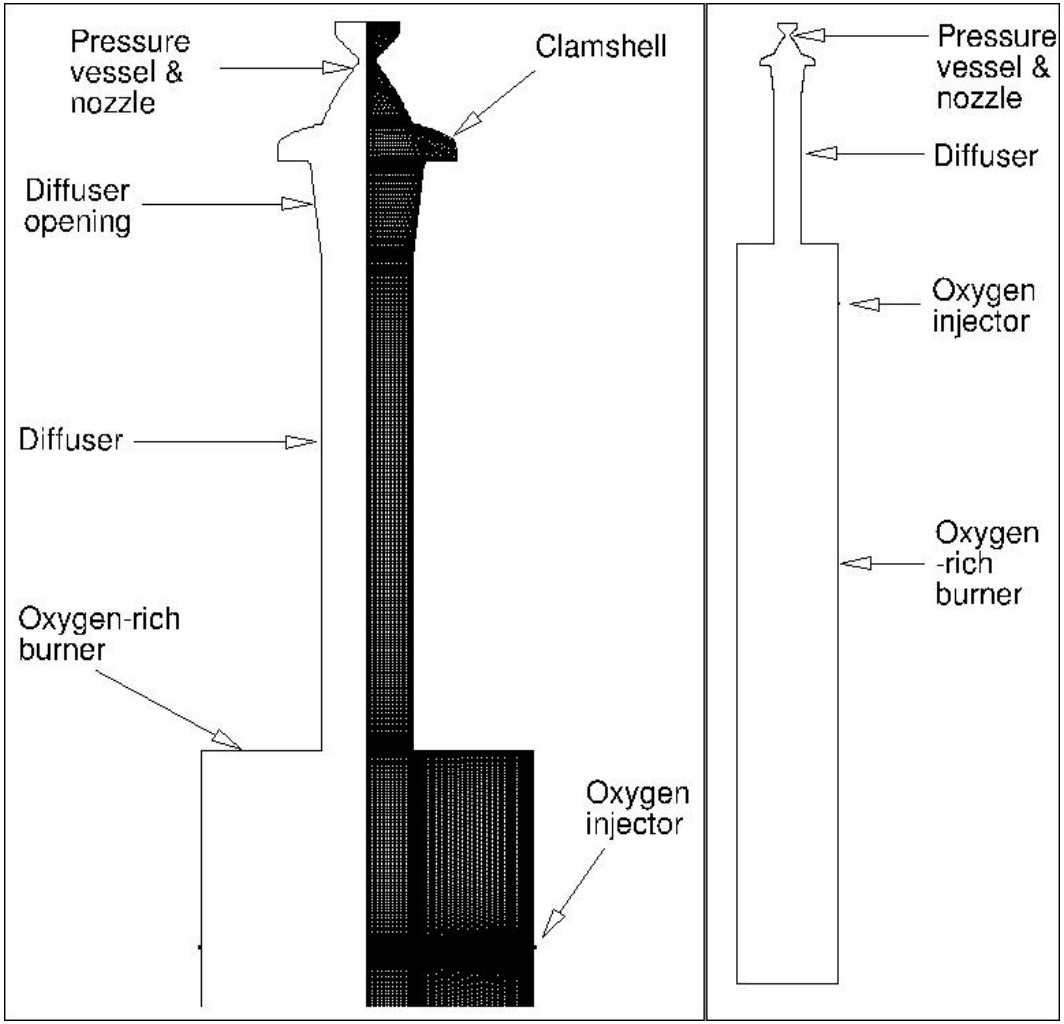
Lower Flammability Limit

The hydrogen and oxygen mixture can not be ignited if the percent of hydrogen in the mixture (less steam) is less than the lower flammability limit (LFL), or higher than the upper flammability limit (UFL). The flammability limits based on the volume percent of hydrogen in oxygen at 14.7 psia (1 atm, 101 kPa) are 4.0 and 94.0 [25]. Converting to mass percent of hydrogen in oxygen, the LFL and UFL are 0.2618% and 49.67%, respectively. Since the idea of the oxygen-rich burner is to burn off hydrogen as much as possible near the end of the burner, UFL is therefore not applicable and the goal is to reduce the mass of hydrogen in dry mixture to a value lower than the LFL. Note that the auto-ignition temperature of hydrogen is 773 deg. K.

The flammability is calculated as:

$$flammability = \frac{\alpha_{H_2} + \alpha_H + \alpha_{OH}(M_H / M_{OH})}{\alpha_{O_2} + \alpha_O + \alpha_{H_2} + \alpha_H + \alpha_{OH}}$$

Axisymmetric Grid & Computational Domain

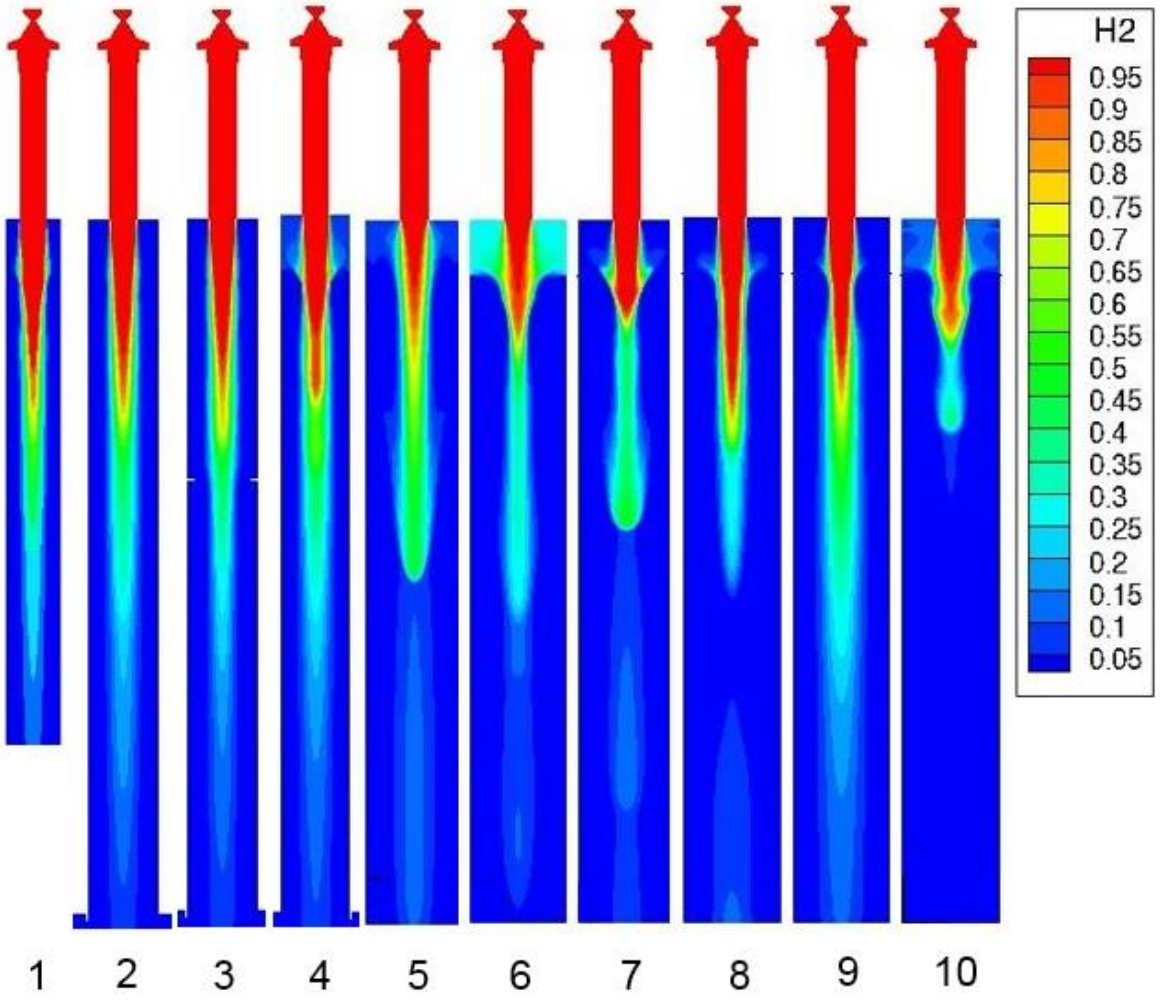


Axisymmetric, Coupled Pressure Vessel & Nozzle/Diffuser/Burner CFD Parametric Studies

Case	O/F	R/R_o	L/L_o	$T_{O2\ inlet}/T_o$	O2 injector geometry	Burner geometry	Ave exit H2 mass fraction, %
1	9	36	705	90	Duct	Straight cylinder	5.81
2	9	46	940	90	Duct	Straight cylinder	3.86
3	9	46	940	90	Duct	Straight cylinder with a long wall fin	3.56
4	9	46	940	300	Sonic nozzle	Straight cylinder	4.27
5	9	65	940	90	Duct	Straight cylinder	3.92
6	9	65	940	200	Duct	Straight cylinder	3.61
7	9	65	940	200	Sonic nozzle	Straight cylinder	4.46
8	9	65	940	300	Sonic nozzle	Straight cylinder	2.58
9	9	65	940	300	Swirled sonic nozzle	Straight cylinder	5.84
10	12.5	65	940	300	Sonic nozzle	Straight cylinder	0.96

This CFD parametric study results show the importance of inter-connected physics such as turbulent mixing, finite-rate chemistry, and residence times that are driven by design parameters such as geometry, O/F ratio, and state of oxygen. It also shows the importance of having a CFD-based process design such that achieving the design objective of the specialized process could be simulated and demonstrated.

Comparison of H2 Mass Fraction Contours in Coupled Pressure Vessel & Nozzle/Diffuser/burner CFD Parametric Study



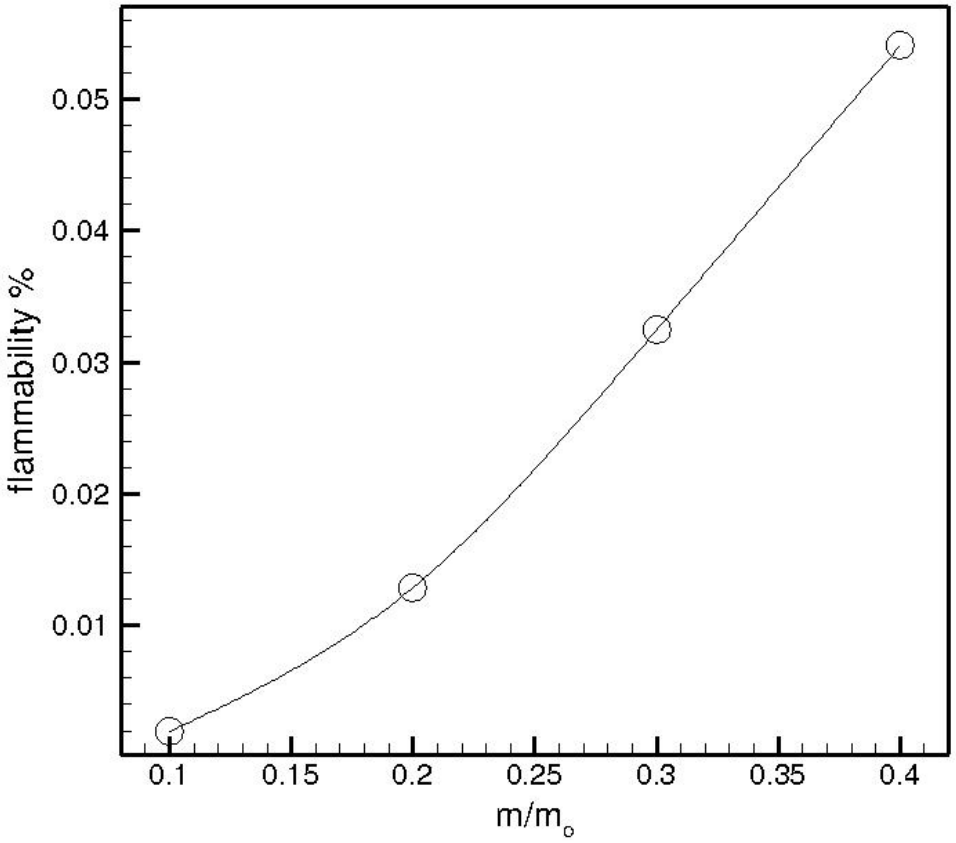
A Heat Exchanger Sizing Result for a Fixed Cooling Tube Diameter

Case	A	B	C	D
$\dot{m}/\dot{m}_o$	1.00	0.50	0.10	0.05
T_{in}/T_o	3,331	3,331	3,331	3,331
T_{out}/T_o	1,053.5	947.1	733.1	658.0
T_{wall}/T_o	400	400	400	400
D/D_o	0.1016	0.1016	0.1016	0.1016
L/L_o	14.732	14.732	14.732	14.732
Re_{in}	114,969	57,485	11,497	5,748
Re_{out}	286,453	156,883	39,410	21,771
$Mach_{in}$	0.568	0.284	0.057	0.028
$Mach_{out}$	0.283	0.130	0.023	0.011
L/D	145.0	145.0	145.0	145.0

Case C is chosen as a nominal case for the demonstrative computation among many possible cases. The heat exchanger sizing tool is a fast, one-dimensional thermal system model. Although more physics have been added, it still uses assumptions such as equilibrium chemistry. To be conservative and considering those assumptions, the actual L/D designed was therefore increased from 145 to 230.

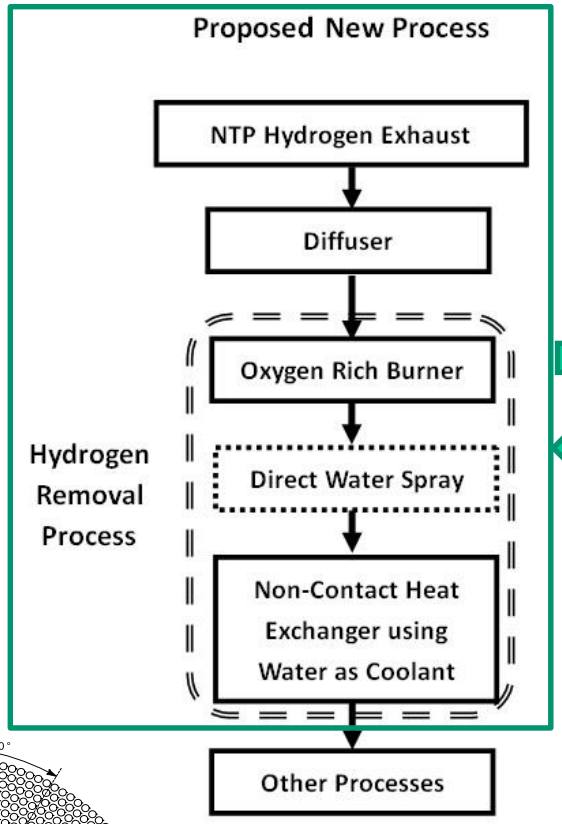
Axisymmetric, Integrated Pressure Vessel & Nozzle/Diffuser/Burner and Single Cooling Tube CFD Results

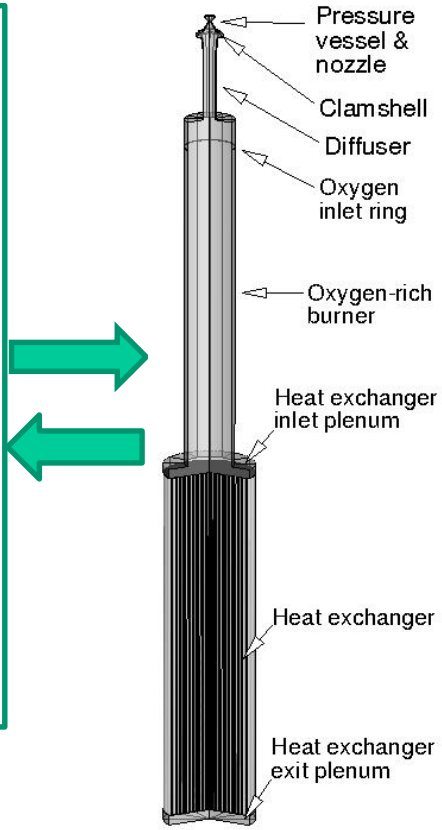
Case	O/F	$\dot{m}/\dot{m}_o$	Flammability %	Flammability % < LFL?
1	12.5	0.1	0.00193	Yes
2	12.5	0.2	0.01288	Yes
3	12.5	0.3	0.03247	Yes
4	12.5	0.4	0.05406	Yes



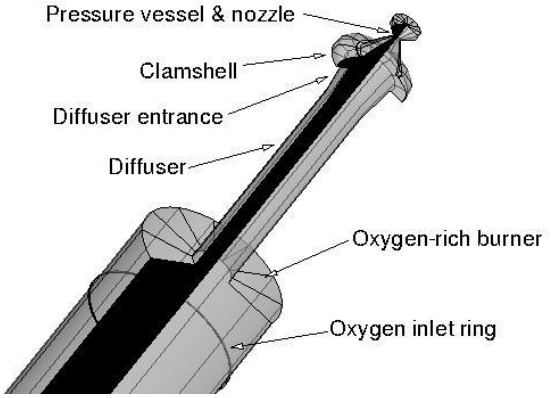
LFL = 0.2618%

3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results

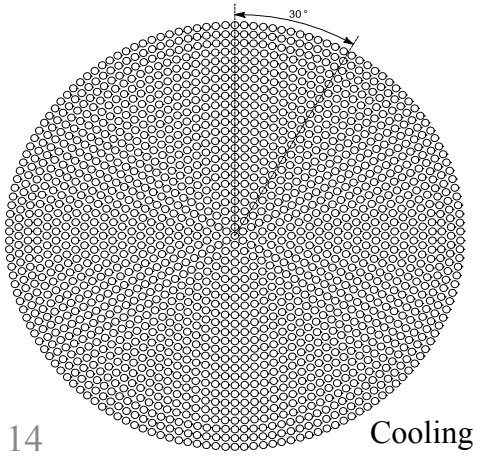




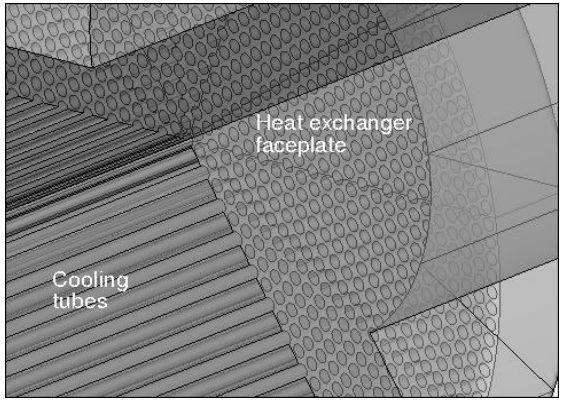
A CFD-based New Process



A close-up view of the layout of NTP engine, nozzle, clamshell, diffuser, and oxygen-rich burner

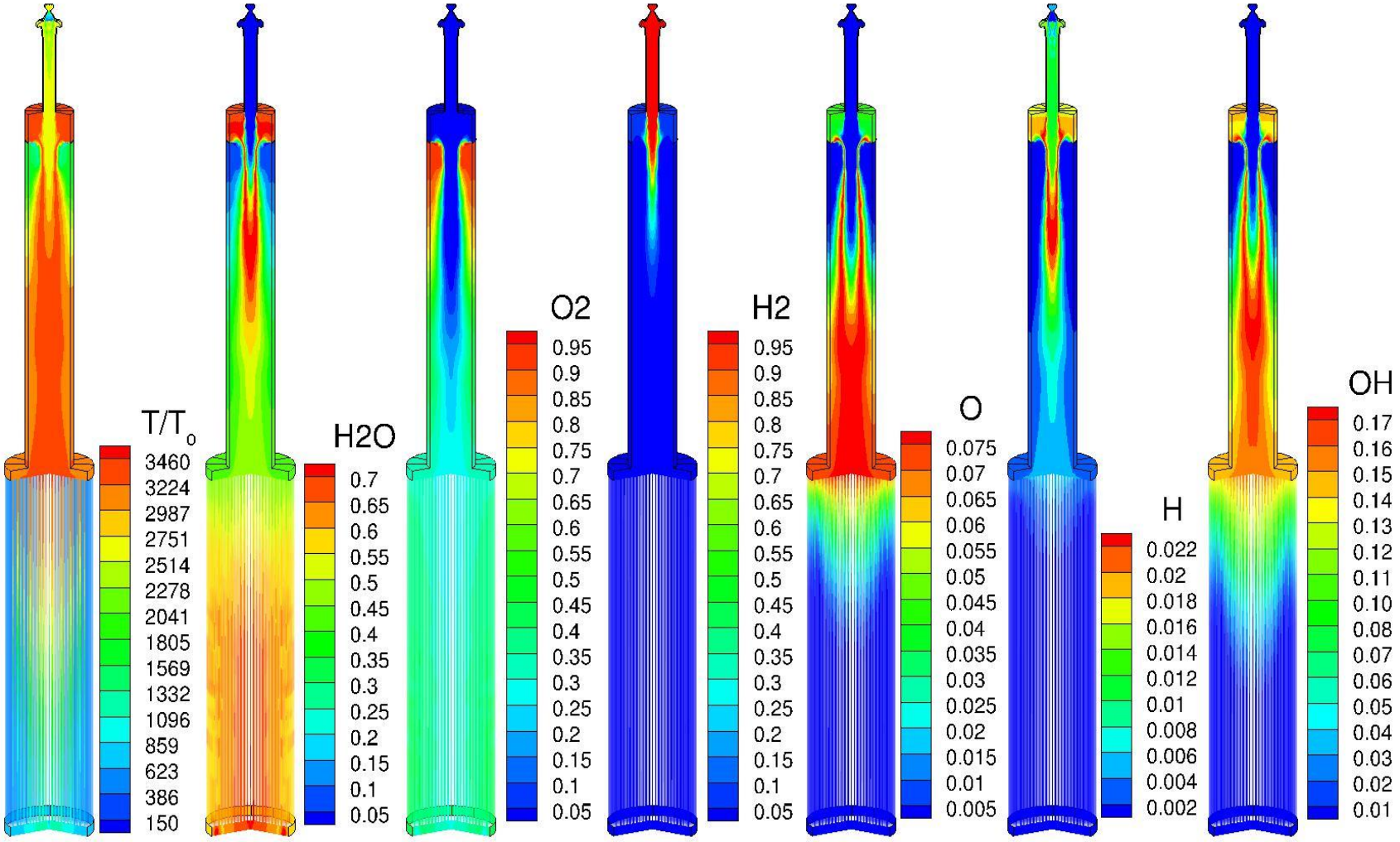


Cooling tubes layout



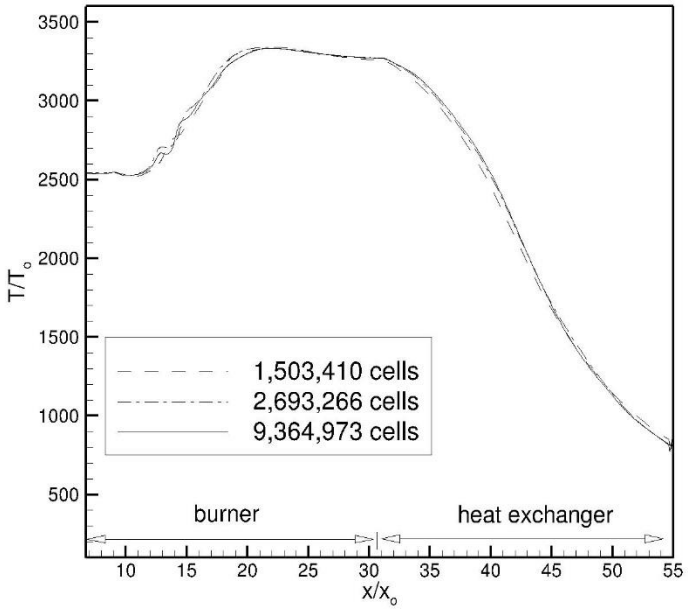
A close-up view of the layout of heat exchanger faceplate and cooling tubes

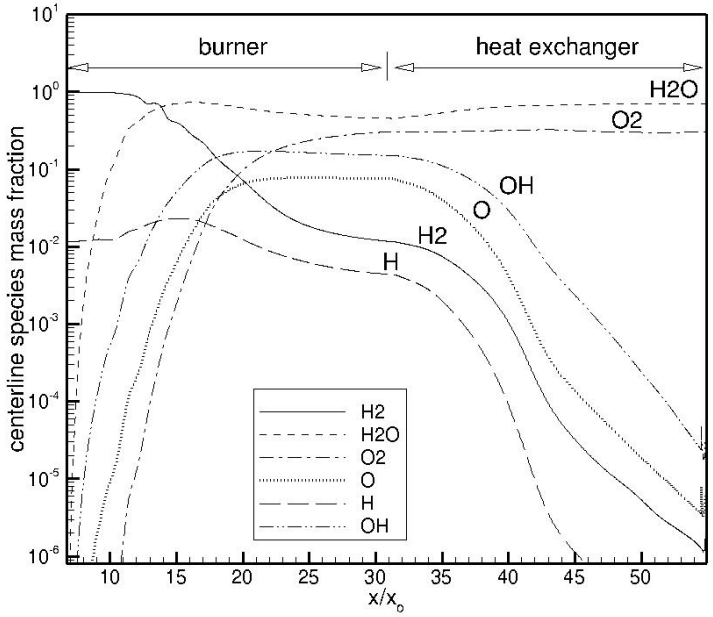
3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results



Computed temperature and species concentration contours on the symmetry plane for the entire three-dimensional process

3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results





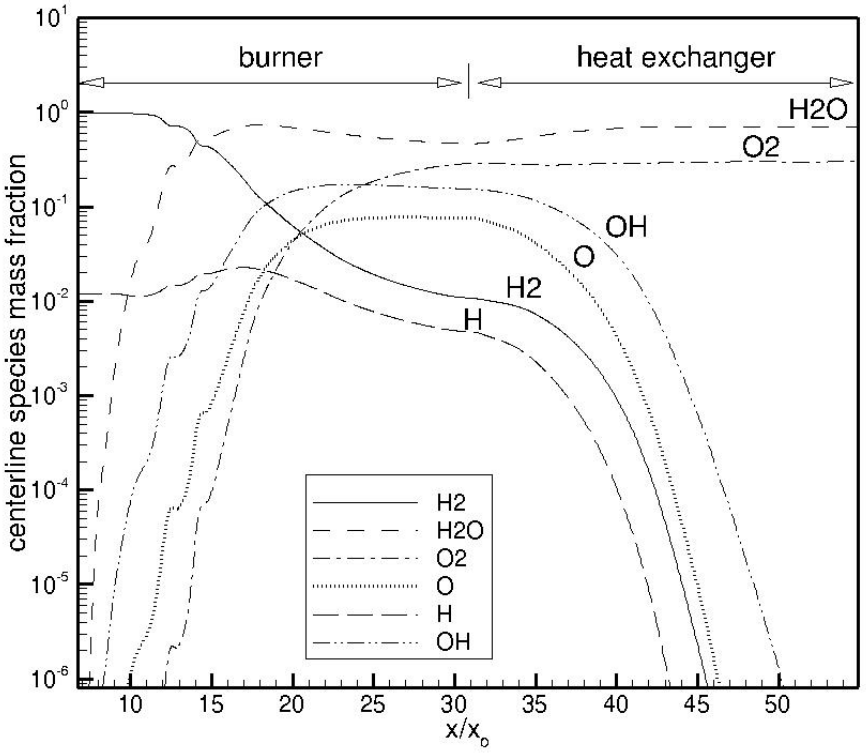
Likely recombination reactions in heat exchanger:

OH + H2 = H2O + H
OH + OH = O + H2O
H + OH = H2O

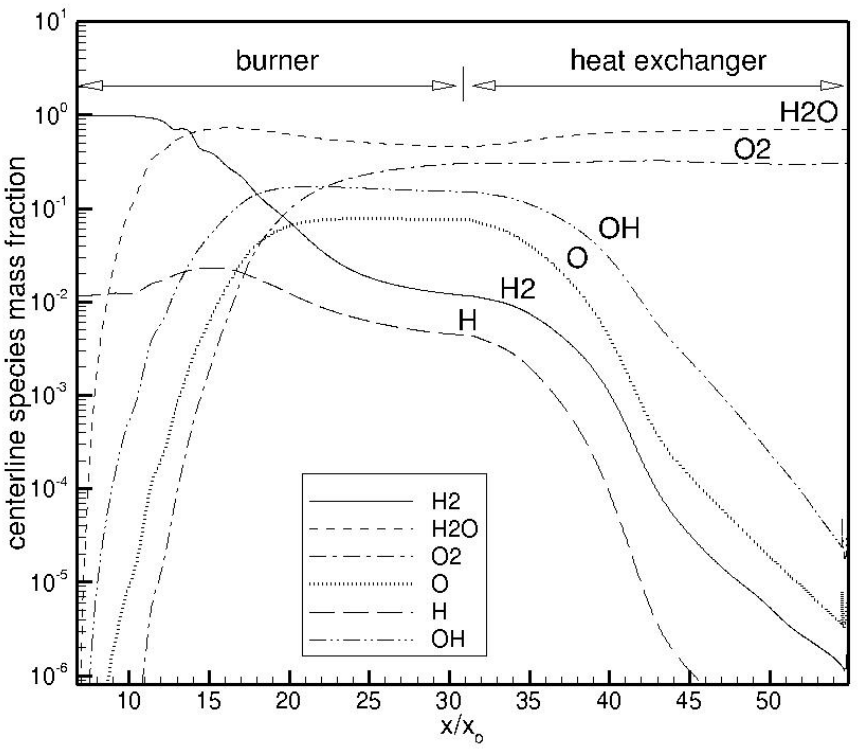
Final flammability computed at the exit plane of the heat exchanger from three grid cell sizes. The flammability results show that H2 total containment objective has been met with the proposed process.

Case	Cell numbers	Flammability %	Flammability % < 0.2618%?
1	1,503,410	0.00300	Yes
2	2,693,266	0.00204	Yes
3	9,364,973	0.00199	Yes

3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results



Equilirbium chemistry



Finite-rate chemistry

3-D, Coupled Pressure Vessel & Nozzle/Diffuser/Burner/Heat Exchanger CFD Results

A comparison of species mass fractions and flammability at end of heat exchanger

species	Finite-rate chemistry	Equilibrium chemistry
H_2	0.34568E-05	0.80734E-11
H2O	0.69773	0.70294
O2	0.30213	0.29706
O	0.12130E-04	0.27250E-10
H	0.15387E-06	0.54466E-15
OH	0.12058E-03	0.17619E-06
Flammability %	0.00199	9.0070E-06

Equilirbium chemistry assumes infinite residence time by assuming infinite reaction rates. Result shows the importance of residence times.

Conclusions

- A computational fluid dynamics based hydrogen containment process is proposed using a non-contact heat exchanger in lieu of direct water spray for better cooling efficiency and recyclable water (without the need for storing a large amount of water).
- The computed flammability at the end of heat exchanger is less than that of the lower flammability limit, demonstrating the total hydrogen containment capability of the proposed process.