

ASSESSMENT OF THE USE OF H<sub>2</sub>, CH<sub>4</sub>,  
NH<sub>3</sub> AND CO<sub>2</sub> AS NTR PROPELLANTS

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Abstract

In this paper the effect of changing from the traditional NTP coolant, hydrogen, to several alternative coolants were studied. Hydrogen is generally chosen as an NTP coolant, since its use maximizes the specific impulse for a given operating temperature. However, there are situations in which it may not be available or optimal. The alternative coolants which were considered are ammonia, methane, and carbon dioxide. A particle bed reactor (PBR) generating 200 MW and cooled by hydrogen was used as the baseline against which all the comparisons were made. Both 19 and 37 element cores were considered. The larger number of elements was found to be necessary in the case of carbon dioxide. The coolant reactivity worth was found to be directly proportional to the hydrogen coolant content.

It was found that due to differences in the thermophysical proportions of the coolant that it would not be possible to use one reactor for all the coolants. The reactor would have to be constructed specifically for a coolant type.

INTRODUCTION

Nuclear Thermal Rocket (NTR) engines are traditionally thought of as using liquid hydrogen as a propellant. This is the preferred propellant, since, for any given exhaust temperature, it results in the highest possible specific impulse. (Approximately twice that of the best chemical rocket). However, there are situations when other propellant types are more desirable, i.e.

1. non-cryogenic storage and handling,
2. availability,
3. safety, and
4. mission optimization.

Furthermore, since an NTR does not require a combustible mixture, the possible propellant types are large and can include such diverse fluids as water, octane, ammonia, methane, carbon monoxide, etc. In the following study, four propellant types were studied. This study considers the physics, fluid dynamics, heat transfer, and materials implications of these propellants. Changes to the baseline design were suggested, and where possible, solutions are suggested. The four propellants chosen for this study are hydrogen (H<sub>2</sub>), methane (CH<sub>4</sub>), carbon dioxide (CO<sub>2</sub>), and ammonia (NH<sub>3</sub>). These propellants cover the range from reducing (H<sub>2</sub>) to oxidizing environments (CO<sub>2</sub>), high hydrogen content (NH<sub>3</sub> and CH<sub>4</sub>) to no hydrogen content (CO<sub>2</sub>) and finally the last three all dissociated in the core. In this manner, the problems and suggested solution should cover other propellants with similar chemical and physical properties.

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A basic requirement of an NTR is that its coolant is initially liquid and then changes to a gas at the exhaust. This implies that the phase of the coolant changes as it passes through the system. It is important that this phase change does not take place within the reactor since it would lead to major control problems. In order to satisfy this requirement, the reactors are operated at pressures that are high enough to ensure that the reactor outlet pressure is beyond the critical pressure for the coolant. In this way, the fluid from the pump outlet to the reactor outlet is all a single phase and no sudden phase change takes place in either the moderator or core. Physical properties for the four coolants to be considered in this study are given below on Table 1. It should be noted that most of the properties are specific to a Particle Bed Reactor (PBR) based design, with properties appropriate to the inlet of the cold frit.

In the following sections, the reactor model will be described. This will be followed by three sections in which preliminary thoughts on physics, fluid dynamics, and heat transfer and material compatibility issues will be discussed.

TABLE 1. Coolant Properties at Cold Frit Inlet

PROPERTY	COOLANT TYPE			
	H <sub>2</sub>	NH <sub>3</sub>	CO <sub>2</sub>	CH <sub>4</sub>
CRITICAL PRESSURE (MPa)*	1.3	11.5	7.4	4.65
CRITICAL TEMPERATURE (K)*	33.2	405.5	304	190.0
TEMPERATURE (K)	100.0	340.0	300.0	220.0
PRESSURE (MPa)	7.0	15.0	10.0	10.0
ENTHALPY (KJ/Kg)	1314	1323	288	-410
VISCOSITY (Kg/ms)	4.2(-6)	1.20(-5)	4.5(-5)	N/A
DENSITY (Kg/m <sup>3</sup> )	17.0	90.4	176.2	88.2
NUMBER DENSITIES (atm/b-cm)	H- 1.0(-2) ----	H- 9.6(-3) N- 3.2(-3)	C- 2.4(-3) O- 4.8(-3)	C- 3.3(-3) H- 1.3(-2)
THERMAL ABSORPTION CROSS SECTION (cm <sup>-1</sup> )	3.3(-3)	9.11(-3)	8.0(-6)	4.3(-3)
THERMAL SCATTERING <sup>†</sup> CROSS SECTION (cm-1)	2.1(-1)	.57(-1)	3.0(-2)	7.2(-1)
SLOWING DOWN POWER ( $\xi\Sigma_s$ )	2.1(-1)	1.9(-1)	9.0(-3)	2.6(-1)

<sup>†</sup> Approximate values since scattering law data does not exist for these molecules.

\*Not at cold frit inlet.

## MODEL

The reactor design to be used in this study is based on the one used in the 200 MW orbital transfer vehicle NTR. This NTR was based on the well known PBR concept described in Reference 1. Two reactor designs based on the 200 MW power level were considered in this study. The design differed primarily in the number of fuel elements. Given below are the basic reactor parameters for the two designs.

TABLE 2. Reactor Design Parameters

PARAMETER	DESIGN 1	DESIGN 2
POWER (MW)	200	200
BED POWER DENSITY (MW/l)	10	10
NUMBER OF ELEMENTS	19	37
CHAMBER TEMPERATURE (K)	3000	3000
CHAMBER PRESSURE (MPa)	7.0	7.0
HOT FRIT ID (cm)	1.111	1.568
FUEL BED ID (cm)	1.411	2.168
FUEL BED OD (cm)	2.928	3.058
COLD FRIT OD (cm)	3.128	4.258
PLENUM OD (cm)	3.428	4.858
ELEMENT PITCH (cm)	11.125	9.647
CORE DIAMETER (cm)	55.63	67.53
CORE HEIGHT (cm)	58.56	67.53
RADIAL REFLECTOR THICKNESS (cm)	10.0	10.0
TOP AXIAL REFLECTOR (cm)	3.0	3.0
BOTTOM AXIAL REFLECTOR (cm)	5.0	5.0
FUEL PARTICLE OD (microns)	500	500

The materials of construction for both reactors are assumed to be the same and are given below.

TABLE 3. Reactor Materials

COMPONENT	MATERIAL
HOT FRIT	COATED CARBON/CARBON
FUEL	ZrC COATED (U,Zr) PARTICLES
COLD FRIT	Al
MODERATOR	Be (80% DENSE) + COOLANT
RADIAL REFLECTORS	Be (90% DENSE) + COOLANT
UPPER AXIAL REFLECTOR	Be
LOWER AXIAL REFLECTOR	C

PHYSICS ANALYSIS

Physics analyses were carried out to determine the multiplication factor for the two reactor designs described above. These analyses were carried out with and without propellant in order to estimate the propellant worth. Furthermore, since the propellants being studied here are not customarily found in reactors, various approximations were used to represent the molecular binding. In one case, (CO<sub>2</sub>) no approximate model could be used and all the calculations were carried out using a free gas scattering model. Finally, since the worth of CO<sub>2</sub> was so low, several designs are proposed for the reactor cooled by CO<sub>2</sub>.

These determinations were carried out using the MCNP Monte Carlo code. The use of this code makes it possible to explicitly represent all the geometric detail necessary to make an accurate determination of the multiplication factor. Figure 1 shows the schematic representation of a fuel particle, a fuel element embedded in the moderator and both a radial and axial section through a PBR based NTR. In these analyses, the heterogenous nature of this reactor is preserved and all the leakage paths are explicitly represented. Neutron spectral shifts which occur between the moderator and fuel zones are accounted for accurately in this analysis technique. The MCNP code uses point cross sections data from the ENDF/B files and thus avoids the inaccuracies implied by group averaged cross sections.

Table 4 shows the multiplication factor (ke) for various configurations, propellants and scattering models. The average standard deviation in ke is .002.

TABLE 4. Multiplication Factors ( $k_e$ )

CASE	PROPELLANT	NUMBER OF ELEMENTS	RADIAL REFLECTOR THICKNESS	$k_e$
1	—	19	10	.925
2	H <sub>2</sub>	19	10	1.024
3	NH <sub>3</sub>	19	10	1.120
4 <sup>+</sup>	NH <sub>3</sub>	19	10	1.100
5	CO <sub>2</sub>	19	10	.944
6	CO <sub>2</sub>	19	20	1.014
7	—	37	10	1.079
8	CO <sub>2</sub>	37	10	1.098
9	CH <sub>4</sub>	19	10	1.083
10 <sup>+</sup>	CH <sub>4</sub>	19	10	1.067

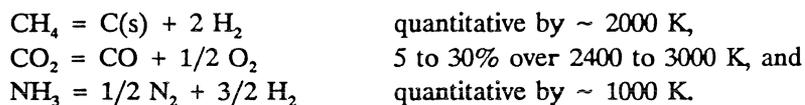
<sup>+</sup>Hydrogen bound in Benzene molecule.

From these results, it is clear that a critical reactor in the size of interest (200 MW) can be designed for all propellants considered in the study. In all cases, except the CO<sub>2</sub> cooled reactor, a 19 element arrangement with a 20 cm thick radial reflector is required. However, in the case of CO<sub>2</sub>, the poor moderating properties of the coolant ( $\xi\Sigma_c$ ) results in a system with a very small coolant worth. Thus, a core which has a sufficiently large value of  $k_e$ , without coolant in it, must be designed. This increase in  $k_e$ , while maintaining the same total power, power density and fissile loading can be achieved by using more fuel elements. An increase in the number of fuel elements, while maintaining all mission performance parameters, makes the core more homogeneous, and thus increases the value of  $k_e$ . Hence, a 37 element core was designed for the CO<sub>2</sub> cooled reactor, and it can be seen that a satisfactory value of  $k_e$  results.

It should be noted that the worth of the coolant is largest for NH<sub>3</sub> and CH<sub>4</sub> ( $.15 < \Delta k < .2$ ), intermediate value ( $\Delta k = .1$ ) for H<sub>2</sub> and the smallest value for CO<sub>2</sub> ( $\Delta k = .02$ ). This variation in coolant worth will impact the start up and control scenarios for the various reactor designs. Furthermore, the concept of using a single reactor design to operate on all the four coolant types is unrealistic. Finally, calculations were carried out to estimate the effect of binding on the hydrogen scattering model. Since neither CH<sub>4</sub> or NH<sub>3</sub> kernels exist, these were approximated by hydrogen as bound in benzene (C<sub>6</sub>H<sub>6</sub>) in the cooler parts of the reactor and unbound (free gas) in the outlet duct. It can be seen that the change in  $k_e$  is approximately .02 for this change in scattering kernel.

#### MATERIAL COMPATIBILITY

At high temperature, all the gases (CH<sub>4</sub>, CO<sub>2</sub>, NH<sub>3</sub>) are unstable at a pressure of approximately 2 MPa.



The use of methane, a common feedstock for pyrocarbon deposition, as propellant is unlikely. It would appear that kinetic hinderance of carbon deposition might prevent this system from clogging or insulating the fuel bed/element.

Carbon dioxide is a possibility if fuel, frit, and ancillary hardware are fabricated from materials compatible with hot  $\text{CO}_2/\text{CO}/\text{O}_2$ . Refractory oxides are an obvious possibility. Information on HTGR particle fuel kernels of  $\text{UO}_x$  and  $\text{UThO}_x$  exist. Ceramic frits of  $\text{ThO}_2$  (mp\* 3370 C),  $\text{Y}_2\text{O}_3$  (mp 2704 C),  $\text{MgO}$  (mp 2825 C), and others are possibilities. However, these materials are brittle and their thermal shock resistance is fair to poor.

In the case of ammonia, a "new" materials effort, nitrides for instance, would require examination of the full range of issues: similar to efforts in the  $\text{CO}_2$  system. However, nitrides are generally less stable and have lower melting temperature than their oxide or carbide counterparts. While oxides are most likely unstable in the hot  $\text{N}_2/\text{H}_2$  ( $\text{H}_2$  being the concern), certain metal carbides might resist hot  $\text{N}_2/\text{H}_2$ ; i.e. TaC. Thus, alternatively, an assessment of the stability of refractory metal carbides in hot  $\text{H}_2/\text{N}_2$  should be pursued.

Finally preliminary thermochemical calculation indicate TaC stability in hot CO, however, compatibility must be shown to exist with other materials, and the potential for carbon deposition in the nonisothermal reactor environment must be explored.

#### FLUID DYNAMICS AND HEAT TRANSFER

Detailed fluid dynamics and heat transfer calculations of these reactor designs have not been carried out at this stage. However, the following preliminary insights into potential design changes can be made.

1. The high value of specific heat for hydrogen compared to the other coolants indicates a much lower mass flow rate for hydrogen to extract the same power. This lower mass flow will result in a lower thrust rocket, despite the higher value of specific impulse.
2. The lower value of viscosity for hydrogen has implications in pressure drop determinations. This is particularly true in the case of the cold frit, whose pressure drop is a strong function of coolant viscosity. This is the primary fluid dynamic reason why one reactor cannot be used with different propellant types; and
3. The much higher density for  $\text{NH}_3$ ,  $\text{CO}_2$ , and  $\text{CH}_4$  somewhat off-sets the lower value of specific heat compared to hydrogen. Thus, the higher mass flow rates required for these coolants may be accomplished through similarly sized coolant passages, i.e. moderator, pressure vessel, etc.

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mp = melting point

## CONCLUSIONS

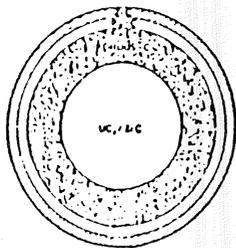
The following conclusions can be drawn from this preliminary study.

1. The use of alternative coolants in a PBR based NTR does not pose any insurmountable physics problems. Those coolants with the highest hydrogen content will require care in design in order to minimize the reactivity swing associated with startup.
2. The excellent heat transfer characteristics typical of a PBR ensure that the fuel particles will always be coolable, even in the cases where the thermophysical properties are less desirable than those corresponding to hydrogen.
3. Chemical and material compatibility problems would seem to imply the largest amount of effort in order to make the use of alternative propellants practical.
4. Finally, due to its high power density and the small size, the PBR would be the ideal system to design especially using a coolant available at the mission destination. Such a system could be carried along as part of the payload and could then be used at this destination.

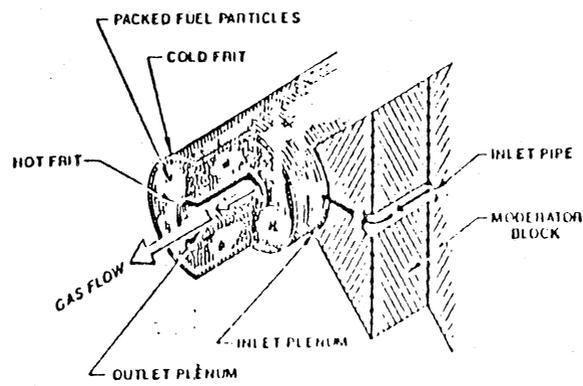
## References

1. J. R. Powell et al., "Nuclear Propulsion Systems for Orbit Transfer Based on the Particle Bed Reactor," 4th Symposium on Space Nuclear Power Systems, Albuquerque, NM, Jan. 1987.

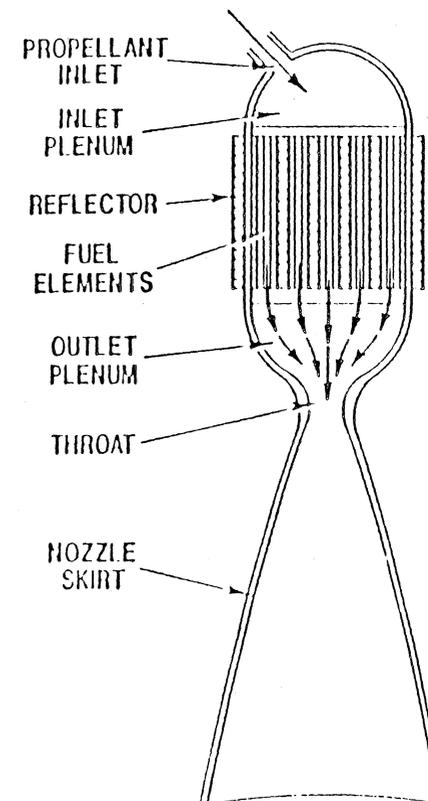
### FUEL PARTICLE



### BASELINE FUEL ELEMENT & MODERATOR BLOCK



### ROCKET



1. Schematic Representation of a Particle Bed Reactor Based Rocket Concept.