

## A Suggestion of the Hydrogen Flame Speed Correlation under Severe Accidents

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### 중대사고시 수소연소에 의한 화염속도 상관식 제시

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#### Abstract

The flame speed correlation considering thermal-hydraulic phenomena under severe accidents is proposed and correction coefficients are defined. This correlation modifies the pressure dependency in Iijima-Takeno correlation and adds the steam suppression effects to it in the anticipated hydrogen and steam concentration ranges under severe accidents. The existing models of flame speed due to hydrogen combustion under severe accidents are based on the experiments which were performed merely at room temperature and atmospheric pressure. They have difficulty in predicting a accurate flame speed in a case of high temperature and pressure during severe accidents.

Thus the flame structure is assumed as a prerequisite to the reliable determination of flame speed and theoretical model is developed. To examine the validity, flame speeds in various conditions calculated by this model are compared with those obtained by the calculation of the existing correlations of the codes such as improved HECTR and MAAP. Also the steam suppression ratio is quantified and the steam suppression coefficient is defined as a composition of mixture. Initial temperature and pressure dependencies are investigated and correction coefficients are determined. More experimental studies can be recommended to improve this correlation to its further works.

#### 요 약

중대 사고시 고온·고압의 열수력적 현상과 증기의 억제효과를 정량화할 수 있는 수소연소에 의한 화염속도 상관식을 제시하고 보정인자들을 정의하였다. 이 상관식은 기존의 Iijima-Takeno 상관식에 중대사고시에 예상되는 수소와 증기의 농도 범위에서 증기의 억제효과를 정량화하는 인자인 증기억제율을 정의하여 추가하고, 초기 압력의 영향을 고려하는 보정효과를 변형한 것이다. 또한 기존의 화염속도 모델은 상온·대기압력에서 수행된 실험에 기초한 상관식으로 중대사고시의 고온·고압의 열수력적 현상을 올바르게 모사할 수 없으며, 증기의 억제 효과를 정량화할 수 없었다.

따라서 화염의 구조를 정의하고, 해석적 분석을 통해 화염속도를 계산하였고, 이 결과를 중대사고 해석용 코드인 MAAP, HECTR의 상관식 결과와 FITS 실험자료와 비교하여 해석적 모델의 적합성을 검증하였다. 이러한 결과를 기초로 화염속도에 대한 증기의 억제효과를 정량화하고, 초기 온도와 압력의 영향을 보정하는 인자들을 결정하여 수소연소에 의한 간편한 형태의 화염속도 상관식을 제시하였다.

## 1. Introduction

The behavior of the potentially large quantity of hydrogen generation during severe accidents has been recognized as an important issue that might pose threats to containment integrity since the accident at Three Mile Island.

The TMI accident resulted in the generation of an estimated 150 to 600 kg of hydrogen, some of which burned inside the containment building, causing a transient pressure rise of roughly 200kPa. For large dry PWR containments, even 100 zirconium oxidation is expected to lead hydrogen mole fraction to be in the range from 10 to 14 in the absence of steam concentration.

The combustion is a rapid chemical reaction accompanied by release of heat and emission of light. The main concerns with hydrogen combustion during severe accidents are the thermal load and pressure load to the containment. One of the important characteristic parameters that have a great influence on pressure load is flame speed, which is required to calculate pressure and temperature transients due to combustion. Faster burning process will produce higher combustion gas pressure and temperature because there will be less amount of heat lost to surfaces. On the contrary, slower flame speed will result in a lower peak combustion pressure and temperature because more heat is lost to surfaces.

The existing models of flame speed are based on experiments, which were performed merely at room temperature and atmospheric pressure. They have difficulty in predicting an accurate flame speed in a case of high temperature and pressure

in which severe accidents proceed.

From this point of view, the objectives of this paper are to develop the model of flame speed due to hydrogen combustion by theoretical analysis and compare these results with those obtained by calculation of existing codes such as improved HECTR and MAAP in order to examine the validity. And the effects of steam in the unburned gas on the flame speed is quantified and the steam suppression ratio (or steam suppression coefficient) is defined in terms of a composition of mixture.

Finally the flame speed correlation considering high temperature dependency, high pressure dependency and steam effect is proposed and correction coefficients are determined.

## 2. Theoretical Analysis

### 2.1. Burning Velocity

The flame is the result of a self-sustaining chemical reaction usually made visible by luminosity of the burning gases. Combustion occurs in a gas mixture composed of fuel and oxidant(oxygen in the air) uniformly. In ordinary deflagration, flame speed is sufficiently subsonic that spatial gradients may be neglected. One-dimensional energy balance equation in steady state is described as follows assuming that radiation, viscous effect, and buoyant effect are disregarded and that  $Le$ , Lewis number is unity.

$$\lambda \frac{d^2 T}{dx^2} - C_p \rho S_u \frac{dT}{dx} + \dot{Q}_w = 0 \quad (1)$$

where  $\lambda$  : thermal conductivity  
 $C_p$  : specific heat capacity  
 $\rho$  : hydrogen density  
 $S_u$  : burning velocity  
 $Q$  : heat of combustion  
 $\omega$  : reaction rate

As a prerequisite to the reliable determination of flame speed, it is necessary to have some assumptions in flame structure. The flame structure is assumed to be divided into three regions, referred to as the preheat zone, reaction zone and burned gas zone. Figure 2.1 illustrates the flame structure regime for a premixed hydrogen laminar flame wave.

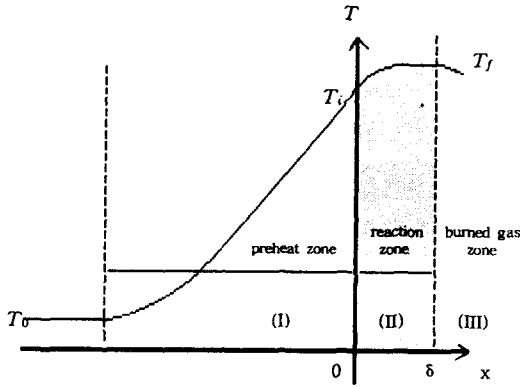


Fig. 2.1. Temperature Regimes in a Laminar Flame

where  $T_0$  ; initial temperature  
 $T_i$  ; ignition temperature  
 $T_f$  ; flame temperature

The combustion reaction is considered to occur in an interface, which is called flame front, between preheat zone and burned gas zone. In flame front, which is taken as an indication of the progress of the flame, the unburned gas is converted into the products. The reaction rate is expressed in the Arrhenius form to yield the first order reaction, which is one step kinetics. The

unburned gas is heated to ignition temperature in a preheat zone in which the conduction and convection heat transfers are dominant and the reaction process can be negligible.

Thus in the preheat zone I in figure 2.1 the energy equation is written as

$$\lambda \frac{d^2 T}{dx^2} - C_p \rho S_u \frac{dT}{dx} = 0 \quad (2)$$

with boundary conditions :

$$T(-\infty) = T_0 ; T(0) = T_i \quad (3)$$

The reaction zone II extends to a small distance  $\delta$ , so that in this zone the energy balance equation is written as

$$\lambda \frac{d^2 T}{dx^2} + wQ = 0 \quad (4)$$

with the boundary conditions :

$$T(0) = T_i ; T(\delta) = T_f \quad (5)$$

The additional condition, which permits the determination of the burning velocity, is the requirement of the continuity of heat flow at the interface between preheat zone and reaction zone.

$$\lambda \left( \frac{dT}{dx} \right)_{x=0,I} = \lambda \left( \frac{dT}{dx} \right)_{x=0,II} \quad (6)$$

Thus we can derive burning velocity,  $S_u$

$$\begin{aligned} S_u &= \frac{1}{\rho} \left[ \frac{2\lambda Q}{c_p^2 (T_i - T_0)^2} \int_{T_i}^{T_f} \frac{dT}{T} \right]^{1/2} \\ &= \frac{1}{\rho} \left[ \frac{2\lambda Q}{c_p^2} \frac{(T_f - T_i)}{(T_i - T_0)^2} \right]^{1/2} \end{aligned} \quad (7)$$

where

$$w = \frac{1}{T_f - T_i} \int_{T_i}^{T_f} \frac{dT}{T} \cdot dT$$

## 2.2. Flame Speed

Conventionally, the term is used "burning velocity" when referring to the rate of burning with

respect to the flame front, i.e., the propagating velocity relative to the moving unburned gas ahead of the flame front. And the term "flame speed" is used when referring to burn rates as measured in the laboratory coordinate system.

The relation between burning velocity and flame speed in an one dimensional premixed laminar flame is illustrated in figure 2.2.

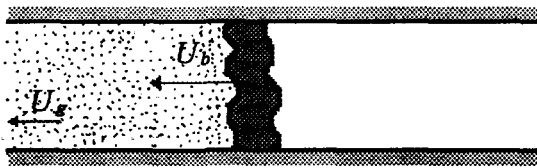


Fig. 2.2 Relation Between Burning Velocity and Flame Speed

where  $S_u = U_b - U_g$

$S_u$  : burning velocity

$U_b$  : flame speed

$U_g$  : unburned gas mixture speed ahead of flame

By equating the mass flux of unburned gas in front of the flame front to that of burned gas behind the flame front, the following is obtained :

$$S_u A \rho_u = U_b A \rho_b \quad (8)$$

where

$A$  : cross-sectional area of flame front

$\rho_u$  : unburned gas density

$\rho_b$  : burned gas density

Hence, the flame speed is given as :

$$U_b = \frac{\rho_u}{\rho_b} S_u \quad (9)$$

Therefore the flame speed is larger than burning velocity by the product of the ratio of unburned to burned gas densities, which, at stoichiometric, is about 7.

### 2.3. Adiabatic Flame Temperature

The combustion process is assumed to take place adiabatically and with no work or changes in kinetic or potential energy. For such a process the temperature of the products is referred to as the "adiabatic flame temperature". This is the maximum temperature with no heat transfer that can be achieved for given reactants, because any heat transfer from reacting substances would tend to lower the temperature of the products. Measurements of flame temperature have shown that the translational gas temperature rises linearly and eventually reaches a value comparable to the isenthalpic values calculated using thermodynamics. The flame temperature is found by equating the end state enthalpy to the sum of the initial enthalpy and combustion energy release. Newton's rule is employed to solve for adiabatic flame temperature based on the following equation.

$$H_{g,o} + Q_b = \left[ \sum_{i=1}^3 M_i C_{p,i} \right] T_{g,fl} + M_{st} h_{st}(T_{g,fl}, P_0) \quad (10)$$

where,

$H_{g,o}$  : initial gas enthalpy

$C_{p,i}$  : specific heat capacity at constant pressure

$T_{g,fl}$  : adiabatic flame temperature

$M_{st}$  : steam mass

$h_{st}$  : steam enthalpy

$i$  :  $H_2, O_2, N_2$

### 2.4. Steam Suppression Effects and Temperature-Pressure Dependency

As steam provides an additional heat sink capacity which helps to quench of the flame, it suppresses the flame speed and then affects the final pressure. The steam suppression ratio is defined as a function of hydrogen concentration to quantify its effects on the flame speed. The ratio is one of the characteristic parameters affecting flame speed. It is given as follows :

$$\Gamma(x_{H_2O}) = \frac{U_b(x_{H_2O})}{U_b(dry)} \quad (11)$$

where

$U_b(dry)$ ; flame speed for steam concentration 0%

Also effects of initial temperature-pressure on flame speed are of great importance because severe accidents result in high temperature and pressure. The higher temperature and pressure would tend to increase flame speed. This is mainly due to preheat effect.

From this point of view, the effects on flame speed are quantified and the flame speed correlation over limited ranges of temperature, pressure and steam concentration is proposed.

### 3. Models of Codes used for Analyzing Severe Accidents

#### 3.1. HECTR(Hydrogen Event; Containment Transient Responses)

The HECTR code was developed by SNL(Sandia National Laboratory) under the auspices of the U.S.NRC to evaluate the hydrogen behavior of a containment during severe accidents. The existing correlation in HECTR version 1.5 has difficulty in predicting the flame speed accurately. Thus the new and improved flame speed correlation [4] which is dependent on combustible gas and diluent gas composition is recommended. This correlation has been based on the combined data of NTS (Nevada Test Site), FITS (Fully Instrumented Tests), and VGES (Variable Geometry Experimental System) experiments. It is given as follows.

$$(1) \text{ For } 0 < X_{H_2} \leq 10\% \\ V_f = L^{1/3} \times (23.70 X_{H_2} - 0.862) \\ \times \exp[X_{H_2O}(a + bX_{H_2O})] \quad (12) \\ \text{where } a = -4.877 \text{ and } b = -3.008$$

$$(2) \text{ For } 10 < X_{H_2} \leq 18\% \\ V_f = L^{1/3} \times (1724 X_{H_2}^2 - 267.28 X_{H_2} + 10.996) \\ \times \exp[X_{H_2O}(a + bX_{H_2O})] \quad (13)$$

where  $a = -4.877$  and  $b = -3.008$

(3) For  $18 < X_{H_2} \leq 25\%$

For all cases, use interpolation.

$$(4) \text{ For } 25 < X_{H_2} \leq 35\% \\ V_f = L^{1/3} \times (289.73 X_{H_2} - 33.769) \\ \times \exp[X_{H_2O}(a + bX_{H_2O})] \quad (14)$$

where  $a = -0.641$  and  $b = -18.38$

(5) For  $35 < X_{H_2} \leq 45\%$

For all cases, use interpolation.

$$(6) \text{ For } 45 < X_{H_2} \leq 80\% \\ V_f = L^{1/3} \times (145.07 - 199.62 X_{H_2}) \\ \times \exp[X_{H_2O}(a + bX_{H_2O})] \quad (15)$$

where

$a = -17.279$  and  $b = 18.07$

$V_f$ : flame speed

$L$ : characteristic length

$x$ : mole fraction

#### 3.2. MAAP(Modular Accident Analysis Program)

MAAP code was developed as part of the IDCOR (Industry Degraded Core Rulemaking) program to predict the thermal-hydraulic behavior of a containment during severe accidents. The laminar burning velocity is assumed to be uniform since beginning of the burning. The laminar burning of MAAP has been correlated by Liu and MacFarlane [1,5]. This correlation includes initial temperature and steam effects.

$$S_u(m/s) = [A_1 + A_2(0.42 - X_{H_2}) + A_3(0.42 - X_{H_2})^2] \\ \times T^{[A_4 + A_5(0.42 - X_{H_2})]} \times \exp(A_6 X_{H_2O}) \quad (16)$$

### 4. Results and Conclusion

The model of flame speed is developed by

Table 2.2. Constants for the Liu-MacFarlane Laminar Burning Velocity

constant	$X_{H_2} \leq 0.42$	$X_{H_2} \geq 0.42$
A <sub>1</sub>	$4.644 \times 10^{-4}$	$4.644 \times 10^{-4}$
A <sub>2</sub>	$-2.119 \times 10^{-3}$	$9.898 \times 10^{-3}$
A <sub>3</sub>	$2.344 \times 10^{-3}$	$-1.264 \times 10^{-3}$
A <sub>4</sub>	1.571	1.571
A <sub>5</sub>	$3.839 \times 10^{-1}$	$-2.476 \times 10^{-1}$
A <sub>6</sub>	-2.21	-2.24

theoretical analysis and in order to examine the adaptability its result is compared to those calculated with correlations of improved HECTR and MAAP under the conditions of FITS(Fully Instrumented Tests). For hydrogen in dry air, the ignition temperature is assumed to lie linearly between 800 and 1000K. In Fig.4.1, the results imply that the flame temperature increases linearly from 780 to 1400K with increasing hydrogen concentration and decreases linearly with increasing steam concentration. Then the flame speed is calculated with the obtained flame temperature. According to the Fig. 4.2, Fig. 4.3 and Fig. 4.4 the flame speed increases with increasing hydrogen concentration and in Fig. 4.5 the speed decreases exponentially with the addition of steam regardless of hydrogen concentration, as radioactive isotopes

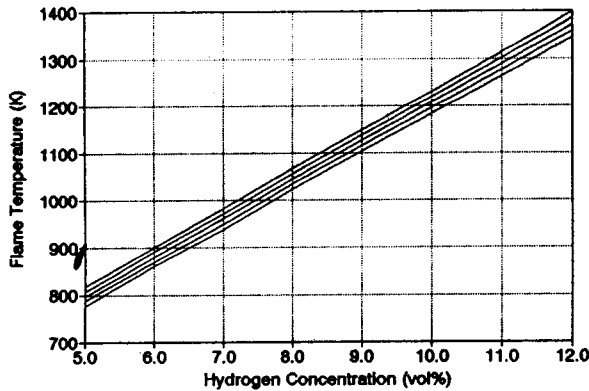


Fig. 4.1. Flam Temperature (Steam Concentration 0,10,20,30,40%)

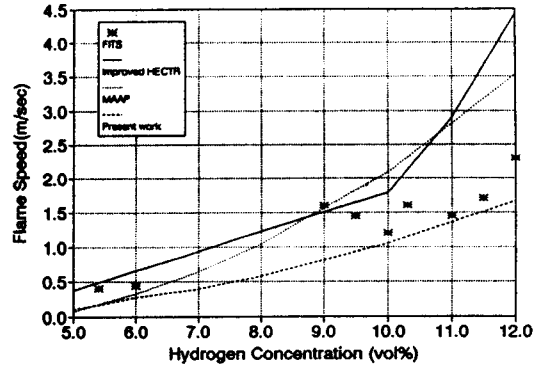


Fig. 4.2. Flame Speed for Steam Concentration 0%

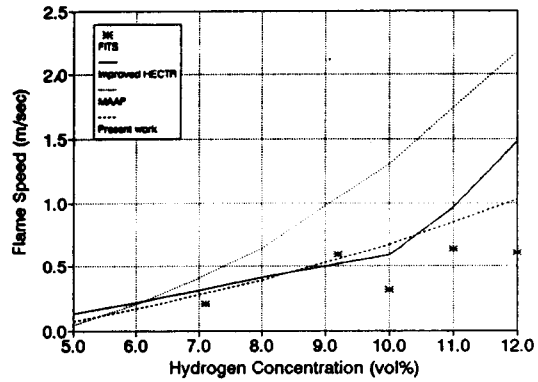


Fig. 4.3. Flame Speed for Steam Concentration 20%

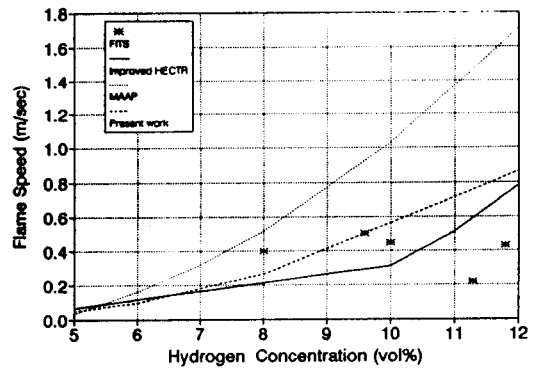


Fig. 4.4. Flame Speed for Steam Concentration 30%

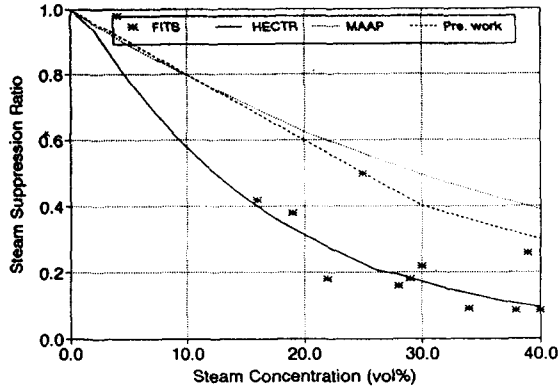


Fig. 4.5. Steam Suppression Ratio for Steam Concentration

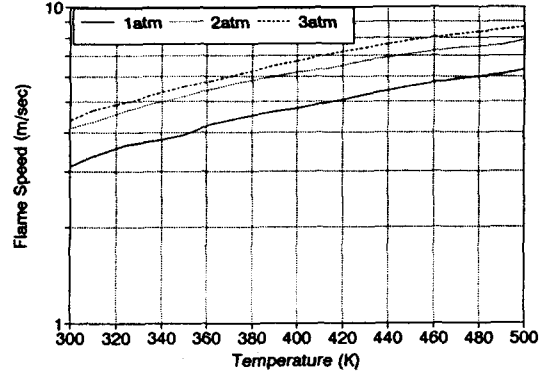


Fig. 4.6. Effects of Temperature for 12% Hydrogen-Dry Air

decay in a given time. If the flame speed is initially  $U_b^0$  in dry air, then at any other vol% steam ( $x_{H_2O}$ ) the flame speed  $U_b(x_{H_2O})$  can be given by an exponential law :

$$U_b(x_{H_2O}) = U_b^0 \exp(-\gamma x_{H_2O}) \quad (17)$$

Here  $\gamma$  is defined as "steam suppression coefficient" which indicates the characteristic of flame speed of hydrogen-air-steam mixtures.

At low steam concentration present work makes a lower prediction than any other calculation of codes. As the steam concentration increases, the present work predicts reasonably.

Usually severe accidents result in high temperature and pressure. However the existing experiments were performed and correlations were developed at room temperature and atmospheric pressure. The higher temperature and pressure would tend to produce higher flame speed.

Thus the effects of temperature and pressure on flame speed are investigated and plotted on the logarithmic scale for hydrogen concentration from 8 to 12%. As examples the presented Fig. 4.6 and Fig. 4.7 represent the effects of temperature and pressure for 12% hydrogen-dry air, respectively. Then flame speed correlation is suggested which can consider high temperature and pressure de-

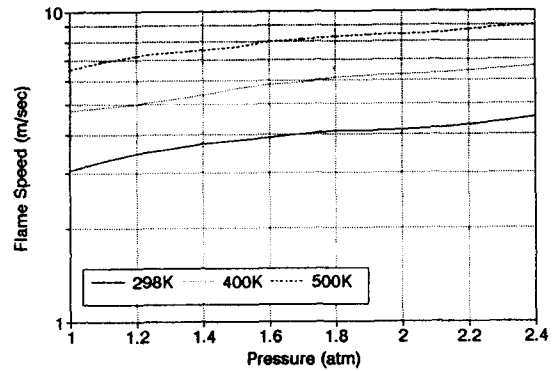


Fig. 4.7. Effects of Pressure for 12% Hydrogen-Dry Air

pendencies, and the correction coefficients are determined on the bases of obtained results. The procedures regarding the temperature, pressure and steam concentration dependencies on flame speed for hydrogen-steam-air mixtures are evidently cumbersome and require more calculation from the theoretical viewpoints.

The suggested flame speed correlation considering initial temperature, initial pressure, and steam effects is given in a simpler form which modifies the pressure dependency in Iijima-Takeno correlation [6] and adds the steam suppression effect to

it.

$$\begin{aligned}
 U_b(x_{H_2}, x_{H_2O}, T, P) & \\
 = U_b^0(x_{H_2}, T_s, P_s) \left(\frac{T}{T_s}\right)^\alpha & \\
 \left[ \beta \ln\left(\frac{10P}{P_s}\right) \right] \exp(-\gamma x_{H_2O}) & \quad (18)
 \end{aligned}$$

where

- $U_b^0$  : flame speed in dry air
- $\alpha$  : temperature correction coefficient
- $\beta$  : pressure correction coefficient
- $\gamma$  : steam suppression coefficient
- $T_s$  : standard temperature (298K)
- $P_s$  : standard pressure (1atm)
- $x$  : mole fraction

The hydrogen- steam- air mixture temperature is varied from 298 to 500 K, the pressure from 1 to 3 atm, and steam concentration up to 40 vol%. In these thermal-hydraulic ranges each coefficient is determined in terms of a range value from the obtained results by method of least squares because the flame speed is dependent on various thermal-hydraulic conditions and has a large uncertainty. Each coefficient ranges in about [1.45, 1.55], [0.40, 0.45], and [2.5, 3.0], respectively. More experimental studies can be recommended to improve this model and to quantify coefficients fully to its further works. Also the improved model which can consider complex characteristics of hydrogen combustion such as geometrical effect, buoyant effect, gravity force, and acceleration will be studied.

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