Modeling the ignition of hydrogen-steam-air mixtures during severe accidents in nuclear power plants

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Abstract

Numerical simulations of the ignition process of hydrogen-steam-air mixtures were performed using a one-dimensional instationary model with detailed chemistry. The mixture composition was varied to cover the range of mixtures expected in nuclear power plants during severe accident scenarios. Minimum ignition energies were determined for mixture temperatures between 300 K and the autoignition temperature. The ignition energies were tabulated for use in multidimensional distribution and combustion simulations on full reactor scale.

Introduction

The design process of next generation nuclear power plants involves the consideration of severe accident scenarios. These accident scenarios involve the release of hydrogen and steam, which originate from inor ex-vessel processes, into the containment, where they mix with air and build a combustible mixture. One of the design requirements for the containment is that it can withstand the expected combustion loads.

The investigation of such accident scenarios involves four distinct phases: the release of the hydrogen/steam mixture into the containment, the distribution and mixing of the hydrogen/steam mixture with air or combustion products from earlier combustion processes, the ignition of the mixture and the subsequent turbulent combustion of the mixed gases possibly with DDT. The distribution and the combustion phase depend strongly on the geometry of the containment and thus require a three dimensional treatment of the geometrical details. While the distribution phase may last several hours the combustion proceeds on a time scale of seconds. This requires the use of different numerical models for the two phases [1, 2, 3].

In this framework an ignition model is needed to determine when to switch from the distribution model to the combustion model. Since the hydrogen/steam mixture enters the containment at high temperatures, the ignition model must cover the self ignition of a hot mixture. We also have to expect hot surfaces and electrical sparks in the containment during the accident and thus must also include the case of such ignition sources. However ignition is a local process and thus we need not consider the geometric properties of the containment.

While several experimental investigations on ignition have been performed (e.g. [4, 5, 6, 7, 8, 9]) these investigations do not cover the whole range of conditions which are needed for reactor applications. Thus a numerical simulation of the ignition process was performed to get more detailed insight into the phenomena involved.

Numerical model

For ignition to occur a sufficiently large pool of chemical radicals must be build before a propagating flame can be established. Thus the details of the chemical kinetics must be considered in the model. For the hydrogen-steam-air mixture we use a reaction schema of Maas and Warnatz [10] with 9 species and 37 elementary reactions.

In our numerical calculations we conservatively neglect turbulence, since during the ignition process turbulence acts primarily to enhance mixing. Thus the energy from the ignition source is distributed over a larger volume resulting in relatively lower temperatures. In addition the mixing also spreads out the chemical radicals needed to establish a propagating flame. As a result the presence of turbulence should reduce the effectiveness of an ignition source. Thus we consider a one dimensional instationary laminar premixed flame in a spherical geometry. The initially homogenous mixture is heated at the center of the computational domain. If the ignition energy is sufficient a laminar flame starts to propagate outward from the ignition source. At the outer boundary of the computational domain a constant pressure boundary condition is assumed. This boundary condition reflects the fact that during the ignition process the state in the containment is not changed.

The numerical calculations were performed with a program developed by U. Maas. The details of the numerical model, the solution procedure and the reaction mechanism are given in [10]. The numerical model solves the conservation equations for mass,

$$\frac{\partial \rho}{\partial t} + \rho^2 \frac{\partial}{\partial \psi} (vr^\alpha) = 0 \tag{1}$$

momentum,

$$\frac{\partial v}{\partial t} + r^{\alpha} \frac{\partial P}{\partial \psi} - \frac{4}{3} r^{\alpha} \frac{\partial}{\partial \psi} (\rho \mu \frac{\partial}{\partial \psi} (v r^{\alpha})) + 2\alpha r^{\alpha} \frac{v}{r} \frac{\partial \mu}{\partial \psi} = 0$$
⁽²⁾

energy

$$\frac{\partial T}{\partial t} - \frac{1}{\rho C_p} \frac{\partial P}{\partial t} - \frac{1}{C_p} \frac{\partial}{\partial \psi} (\rho r^{2\alpha} \lambda \frac{\partial T}{\partial \psi}) + \frac{r^{\alpha}}{C_p} \sum_{i=1}^{n_s} j_i C_{pi} \frac{\partial T}{\partial \psi} + \frac{1}{\rho C_p} \sum \dot{\omega}_i h_i M_i - \frac{4\rho \mu}{3C_p} (\frac{\partial v r^{\alpha}}{\partial \psi})^2 + \frac{2\alpha \mu}{C_p} \frac{\partial}{\partial \psi} (v r^{\alpha - 1}) = q$$
(3)

and species concentrations

$$\frac{\partial w_i}{\partial t} + \frac{\partial}{\partial \psi} (\rho r^\alpha \omega_i V_i) - \frac{\dot{\omega}_i M_i}{\rho} = 0 \tag{4}$$

on a Lagrangian grid using a reaction mechanism with detailed chemical kinetics. Here the generalized coordinate is given by

$$\frac{\partial r}{\partial \psi} - \frac{1}{\rho r^{\alpha}} = 0 \tag{5}$$

Diffusivity of the different species as well as thermo diffusion are fully accounted for. Due to the one dimensional character of the numerical model buoyancy effects had to be neglected.

Results

First test calculations showed that the program works for initial data were ignition occurs as well as for inert cases where the energy is not sufficient to initiate a propagating flame. Figure 1 gives an example of a stoichiometric hydrogen air mixture. In the temperature distribution shown on the left side the heated region in the center of the sphere is clearly observed. The mixture in the core region remains at an almost constant temperature until the ignition delay time is expired. Then the temperature increases



Figure 1: Ignition process in stoichiometric hydrogen air mixture at an initial temperature of 450 K. Temperature distribution (left) and hydrogen mass fraction (right) as function of location and time



Figure 2: Minimum ignition energy as function of temperature

and a flame starts to propagate outward. Behind the flame the hydrogen is completely consumed as can be seen on the right plot. If the ignition energy is reduced below a critical value no propagating flame is observed.

In the next step the influence of the ignition energy, duration of energy deposition and size of energy source were studied. It was found that for realistic ignition source times and sizes the energy density required to ignite the mixture was almost independent of the ignition parameters. Thus only the ignition energy was varied for further investigations of different mixture compositions.

Numerical simulations were performed for a wide range of H_2 and steam concentrations in a temperature range from 300 K to 1000 K. Figure 2 shows the minimum ignition energies required to ignite a given mixture as function of the initial temperature of the mixture. As is expected the minimum ignition energy decreases with increasing initial temperature. At about 900 K the minimum ignition energy drops suddenly to zero. The temperature were this drop occurs is the minimum ignition temperature. Thus the numerical calculations provide information for the evaluation of the effectiveness of ignition sources within the containment as well as for the minimum ignition temperatures where the mixture can be expected to ignite without an additional energy source.

Utilization of Results

To make the numerical results available to the three dimensional distribution and combustion models a local regression model [11] was fitted to the ignition energy data. Subroutines allow access to the data of the regression model and return the minimum ignition energy as function of mixture composition and temperature.

Figure 3 shows results of this fitting procedure for two different initial temperatures. While the results show good agreement for reactive mixtures the fitting procedure does not predict the ignition



Figure 3: Example of fitted data of regression model

limits correctly. At the lean and rich ignition limits the regression model extrapolates the data across the boundary. Here an extension of the fitting procedure is required to improve the model.

Summary

The numerical model of a laminar premixed flame in spherical geometry was able to reproduce the expected dependency of the ignition energy on the initial conditions. However the numerical results show less variation than experimental results. Especially near the flammability limits the criteria used to define ignition are not well defined. Here undocumented details of the boundary conditions in experimental investigations become exceedingly important. This makes it difficult to compare the numerical results quantitatively to experimental findings.

The presented study has demonstrated the predictive capabilities of the numerical code. It will be used in further studies to define conservative data for the self ignition temperature of H_2 -air-steam- N_2 mixtures at accident relevant pressures. Furthermore it is planned to derive conservative ignition limits of these mixtures for various ignition sources (igniters, electrical sparks) in severe accidents. The final result will be an 'ignition module' which can be used in different distribution and combustion codes.

References

- W. Breitung and A. Kotchourko. Numerische Simulation von turbulenten Wasserstoff- Verbrennungen bei schweren Kernreaktorunfällen. Nachrichten- Forschungszentrum Karlsruhe, 28:175–191, 1996.
- [2] P. Royl, E.A. Haytcher, J.R. Travis, and H. Wilkening. Dreidimensionale Simulation von Wasserstoffverteilung und -verbrennung im äußeren Sicherheitsbehälter eines Druckwasserreaktors. Nachrichten- Forschungszentrum Karlsruhe, 28:192–208, 1996.
- [3] J.R. Travis. A heat, mass and momentum transport model for hydrogen diffusion flames in nuclear reactor containments. *Nuclear Engineering and Design*, 101:149–166, 1987.
- [4] A.L. Camp, J.C. Cummings, M.P. Sherman, C.F. Kupiec, R.J. Healy, J.S. Caplan, J.R. Sandhop, and J.H. Saunders. Light water reactor hydrogen manual. Sandia Report SAND82-1137, NUREG/CR-2726, Sandia National Laboratories, 1983.
- [5] H. Tamm, R.K. Kumar, and W.C. Harrosin. A review of recent experiments at WNRE on hydrogen combustion. In *Hydrogen and Water Reactor Safety*, Proceedings of the Second International Conference on the Impact of Hydrogen on Water Reactor Safety, Albuquerque, New Mexico, 1982.
- [6] D.W. Stamps and M. Berman. High-temperature hydrogen combustion in reactor safety applications. In *Thermal reactor safety: Proceedings of the international ENS/ANS conference*, Avignon, 1988.
- [7] R.K. Kumar. Flammability limits of hydrogen-oxygen-diluent mixtures. Journal of Fire Sciences, 3:245–262, 1985.
- [8] R.K. Kumar. Ignition of hydrogen-oxygen-diluent mixtures adjacent to a hot, nonreactive surface. Combustion and Flame, 75:197–215, 1989.
- M. Hertzberg. Flammability limits and cellular flames: Natural convection, flame stretch and selective diffusional demixing. In 1990 Fall Meeting, Western States Section, The Combustion Institute, 1990.
- [10] U. Maas and J. Warnatz. Ignition processes in hydrogen-oxygen mixtures. Combustion and Flame, 74:53–69, 1988.
- [11] W.S. Cleveland, E. Grosse, and M.-J. Shyu. A package of c and fortran routines for fitting local regression models. Technical report, Manual for the software package netlib/a/loess, available at ftp://elib.zib.de/netlib/a/cloess.ps, 1992.