RECOMMENDATION FOR MAXIMUM ALLOWABLE MESH SIZE FOR PLANT COMBUSTION ANALYSES WITH CFD CODES

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Abstract

The selection of the maximum allowable mesh size for a fluid dynamic calculation with CFD codes is essential for the reliability of the results assuming suitable physical and numerical models are used. Calculations with CFD codes are necessary for the assessment of the consequences of pressure loads due to possible hydrogen combustion in nuclear power plants in a severe accident.

CFD simulations of the transport and distribution of the released hydrogen/steam as well as the possible combustion during the transient in the containment require an appropriate mesh size to resolve the relevant phenomena and loads.

The determination of the mesh size has to take into account:

- adequate delineation of the containment geometry for accurate hydrogen distribution calculations,
- sufficient conservative resolution of the combustion phenomena for the determination of pressure wave propagation and pressure loads,
- no loss of pressure wave loads with relevant frequencies for the structural response analysis of the containment during the combustion calculation.

In this paper, it is found that the accuracy of the calculated pressure wave associated with its frequency depends on the mesh size and a simple and easily useable analytical formula for the determination of the maximal allowable mesh size is derived. This formula can be used as a criterion to find out easily and simply the appropriate mesh size for accurate determination of the pressure wave load function. This criterion in form of a relation is deduced in this theoretical treatment from the connection between the structural characteristic associated with the relevant frequency and fluid property associated with mixture quality and gas temperature as well as numerical determination of the pressure wave load function associated with the accuracy of the approximation.

This criterion gives the CFD code users the ability to determine the upper limit of the mesh size during the preparing of the geometry simulation specially for performing a combustion calculation.

The mesh size can be calculated from the analytical formula using:

- the mixture quality and temperature in the cloud confined in the structure (containment),
- the highest relevant frequency for the structural analysis of the containment and
- the number of points for the accurate approximation of the pressure wave function.

1. INTRODUCTION

CFD codes users have always to decide, before starting the fluid dynamic analysis, which relevant mesh size is needed for their calculations. This task is often not simple, e.g. for fast deflagration calculation, the mesh size has to be small enough to resolve all pressure waves relevant for the structural analysis. This can be aggravated by the lack of knowledge of all relevant natural frequencies of the containment structure, which may be under design with the final decision of the characteristics of the structure still being open. In such a case it is of advantage to have a criterion to predict the maximum allowable mesh size for plant combustion analyses with CFD codes without exact knowledge of the structural characteristics.

The appropriate assessment of the consequences of the severe accident pressure loads due to hydrogen combustion in nuclear power plants requires some restriction on the mesh size.

Besides the requirement for:

- minimizing the computer time (→cost reduction),
- minimizing the file sizes (→comfortable visualization and data saving) and
- minimizing the needed man hours (→more time for better assessment of the result and possibility for parametric studies),

additional requirements have to be taken into account for a selection of the mesh size, which plays an important role for the application of the CFD codes for fluid dynamic analysis:

- sufficient delineation of the containment geometry and
- recording of all pressure waves loads with a relevant frequency for the structure response analyses.

This paper describes the method to determine the mesh size for CFD combustion codes, which assumes the correct calculation of the hydrogen distribution as an initial condition for the combustion calculation with the same or other appropriate CFD codes (see Section 2).

In Section 2.1 the characteristics of a multi-degree-of-freedom system is described, which is useful for application of the modal analysis in the dynamic structural analysis for lumped mass system like a containment.

Section 2.2 deals with the relation between the fluid dynamic load function and the structure response, and describes the maximum mesh size and its dependency on the fluid and structure parameters.

The evaluation of the maximum mesh size is shown in Section 3. Also the determined dynamic load factors based on a calculated combustion load for the EPR™ containment are shown in this section.

Section 4 summarizes the results of the theoretical investigation of this report.

2. METHOD

Since an accurate design of the containment structure has many advantages for example reduction of the cost, a dynamic load analysis will be normally used to optimize the containment design with respect to natural frequencies. The application of the results of such analyses can reduce the relevant natural frequencies of the containment due to the possible design of less rigid structures.

These analyses are done in the structural engineering for cases with time dependent loads like:

- moving load (moving crane, or truck over a bridge),
- alternating force (running of an unbalanced engine, starting or stopping of pump),
- force on foundation (earthquake and underground explosion),
- blast wave (internal or external explosion),
- non-periodic load (wind load or aircraft crash) and
- pressure wave and/or shock wave propagation (fast deflagration or DDT inside confinement).

This paper deals with the last item, because its purpose is to determine the upper limit of the mesh size for combustion calculations with CFD codes. The mesh size has to be small enough to resolve all relevant pressure waves as well as their interaction with the structure inside the containment.

Although a continuous structure has an infinite number of degrees of freedom, in practice the use of the finite element method will limit this number.

The structure analyzed here is constituted by internal concrete wall and the containment shell. Thus these structures can be simulated with a large number of elements by using the finite element method, which have a large number of vibration modes. Each possible independent motion of such a system can be described by an independent differential equation of motion associated with a natural frequency of the system.

Each independent motion of the lumped mass can be seen as a natural or normal mode. The number of degrees of freedom is always equal to the number of natural or normal modes.

In cases of continuous mass of the structures like containment structures the system has infinite number of degree of freedom. But in structural engineering the containment structure can be handled as a finite number of lumped masses associated with finite number of natural frequencies.

Each mode of vibration responses applying a pressure load function. However, practically only a limited number of natural frequencies are relevant for the determination of the total response of the structure.

In a structural modal analysis all natural frequencies of a lumped system will be excited with different strength for a given time dependent load function and can respond freely alone. The total response can be found by superposition of the response of each normal mode (see Section 2.1). This means that the complex problem of a multi mode system reduces to a rigorous analysis of each normal mode as an independent equivalent single degree of freedom system.

2.1 **Multi degree of freedom system**

Obviously the total response of the structure is of interest for containment structural analyses.

Since the containment structure can be simulated as a multi degree of freedom system (lumped mass system) associated with a finite number of normal modes and natural frequencies, it is convenient to apply the method of modal analysis from the structural engineering.

In the modal analysis method a multi degree of freedom system will be simulated with a large number of single degree of freedom system (oscillators), one for each relevant mode with corresponding equivalent mass and stiffness coefficient as well as equivalent acting force, respectively.

Each possible independent motion (natural mode of vibration of the system) of the lumped mass system results from exciting of the corresponding natural frequency, that is characteristic for this mode.

Independent differential equations can describe these motions. Each independent motion of the lumped mass can be seen as a natural or normal mode k.

For each mode k this method deduces from the conservation of energy an equation of motion for modal deflection X_k with equivalent mass M_k (modal mass) and equivalent spring constant λ_k (modal stiffness) as system parameters. This equation is similar to the equation of motion for a single oscillator applying an equivalent force $F_{eq}(t)$.

The general form of each mode k can be simulated by a single mass spring system (Norris et al., 1959).

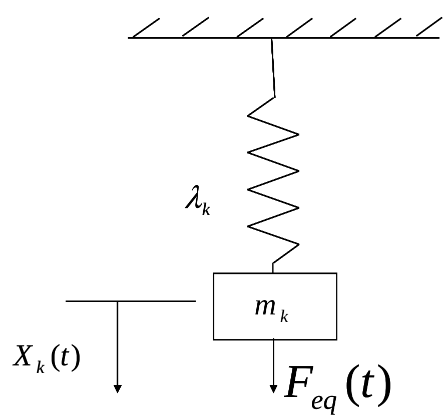

Fig. 1: An equivalent single degree of freedom system without damping for the k th mode.

The differential equation of motion for the modal deflection X_k of the system without damping for the k th mode reads as follows:

$$M_k \ddot{X}_k(t) + \lambda_k X_k(t) = F_{eq}(t)\,, \tag{1}$$

where

M_k: equivalent mass for the k th mode,

λ_k: equivalent spring constant (stiffness coefficient) for the k th mode,

$X_k(t)$: deflection of equivalent mass of the k th mode,

$\ddot{X}_k(t)$: acceleration of equivalent mass of the k th mode,

$F_{eq}(t)$: time dependent equivalent force acting on the k th mode,

with the system parameters for the k th mode:

$$\omega_k = \sqrt{\frac{\lambda_k}{M_k}}: \quad \text{natural circular frequency for the } k \text{ th mode,} \tag{2}$$

$$T_k = \frac{2\pi}{\omega_k} = 2\pi\sqrt{\frac{M_k}{\lambda_k}}: \quad \text{natural time period for the } k \text{ th mode,} \tag{3}$$

$$f_k = \frac{1}{T_k}: \quad \text{natural frequency for the } k \text{ th mode.} \tag{4}$$

From the solution of such a second order ordinary differential equation the response of the above equivalent single oscillator is known.

The solution shows that the maximum deflection of a single-degree-of-freedom system is increased exactly by a factor two if the load appears suddenly (step function) in comparison with an (infinite) slow rise to the same maximum load.

$$X_k^{\max} = 2\,X_k^{static}\,, \tag{5}$$

where

$$X_k^{static} = \frac{Max(F_{eq}(t))}{\lambda_k}\,. \tag{6}$$

A convenient comparison of the dynamic and static deflection of each single degree of freedom system (or of each mode of the system) with and without damping is done in structural engineering by the dynamic load factor (DLF). The DLF is defined as the ratio of time dependent deflection (dynamic deflection) and the constant deflection due to the maximum load as static load:

$$DLF_k(t) = \left|\frac{X_k(t)}{X_k^{static}}\right|, \tag{7}$$

where

$DLF_k(t)$: dynamic load factor of the k th mode,

$X_k(t)$: dynamic deflection of the k th mode due to dynamic load $F_{eq}(t)$ (from the solution of the differential equation of motion for the k th mode),

X_k^{static}: static deflection of the k th mode due to the maximum load $Max(F_{eq}(t))$.

The maximum dynamic stress and deflection are always of interest for the assessment of the structure response, which can be easily determined from the maximal dynamic load factor and static stress and static deflection of each mode, respectively:

$$\sigma_k^{\max} = DLF^{\max}\left(f_k\right)\sigma_k^{static} \tag{8}$$

and

$$X_k^{\max} = DLF^{\max}\left(f_k\right)X_k^{static} \tag{9}$$

where

σ_k^{static}: static stress of the k th mode,

$\sigma_k^{\max}$: maximum dynamic stress of the k th mode,

$X_k^{\max}$: maximum dynamic deflection of the k th mode,

$DLF^{\max}\left(f_k\right)$: maximum dynamic load factor of the k th mode.

By using the definition of the natural circular frequency ω_k, the natural time period T_k and the natural frequency f_k of the mode k, the static deflection X_k^{static} can be written in the following form:

$$X_k^{static} = \frac{Max(F_{eq}(t))}{4\pi^2 M_k f_k^2}\ . \tag{10}$$

This formulation of the static deflection reveals that for equal maximum load and constant equivalence mass the static deflection decreases quadratically for modes with higher natural frequency.

Again the deflection for the mode k is given by applying the dynamic load factor

$$X_k(t) = DLF_k\ (t)\, X_k^{static} \tag{11}$$

It should be mentioned that $DLF_k\ (t)$ is only dependent on the natural frequency for the mode k and non-dimensional equivalent load time function $\dfrac{F_{eq}(t)}{Max(F_{eq}(t))}$.

The maximum dynamic deflection may also be written in terms of the natural frequency using the definition of the static deflection in the corresponding form:

$$X_k^{\max} = DLF^{\max}\left(f_k\right)\frac{Max(F_{eq}(t))}{4\pi^2 M_k f_k^2}\,. \tag{12}$$

This formulation clearly reveals that the higher the normal mode associated with higher natural frequencies f_k of a lumped mass multi degree system is, the lower is the maximum dynamic deflection $X_k^{\max}$ if the achieved $DLF^{\max}\left(f_k\right)$ due to the non-dimensional load stays constant or decreases. In other words, if the DLF for the same non-dimensional load function decreases or stays constant for higher natural frequencies of the system, then the maximum dynamic deflection decreases with the inverse square of the frequency. This is an important fact, because this statement can be also applied for the total maximum dynamic deflection or structure response, which can be found by superposition of their deflections for all modes of the system in structural engineering.

The upper limit of the relevant natural frequency of a multi lumped mass system like a containment can be achieved from the graph of the calculated maximum dynamic load factors acting relevant non-dimensional load functions for all natural frequencies. However, in practice the calculation of the maximum DLF for natural frequencies up to the bounding frequency of 200 Hz for a concrete structure is sufficient (see right panel of Fig. 3). Above this bounding frequency the maximum dynamic deflection for a concrete structure is very small and can be neglected.

The upper limit of the relevant natural frequency of a multi lumped mass system is the frequency from which the calculated maximum DLF up to the bounding frequency stays constant or decreases.

This statement can be used as a criterion to determine the limits of the upper frequency of the given load function up to the bounding frequency of the corresponding structure material, which can be relevant for the structure response.

This statement leads to the desired connection between combustion load and structure response, which is described in the Section 2.2.

It has to be mentioned that the same tendency is valid if the damping of the system is taken into account. In this case the response is smaller and the natural frequency decreases. Thus no significant effect is expected. For a concrete structure at least 4 to 5 % damping should be considered to simulate the concrete characteristic more accurately.

2.2 **Correlation between fluid dynamic combustion load and structural response**

The response of each mode of a multi lumped mass system is massively dependent on the frequency content of the pressure load function. The impact of a pressure wave with a certain frequency is normally higher on the deflection of the mode with the same natural frequency as on the modes with other natural frequencies.

The relevant pressure load function due to combustion can be taken either from:

- relevant experiments, or
- combustion calculations for appropriate scenarios.

In the first case the frequency of the recorded pressure wave and/or shock wave has to be high enough to resolve all waves with relevant frequencies. In the second case the mesh size has to be small enough to resolve all pressure waves and/or shock waves with relevant frequencies during the combustion calculation. Obviously the relevance of resolving the waves up to bounding frequency of the system is clear for both cases.

Recording a pressure wave during an experiment up to very high frequencies is no problem, and usually the resolution of pressure waves during the experiment is sufficient. Recording the frequency content above the bounding frequency of 200 Hz is irrelevant as mentioned in the previous Section 2.1 for a concrete structure and can be filtered from both experimental and calculated pressure wave load functions.

Pressure load functions exist from different combustion experiments for different gas mixtures and different geometries.

When using experimental results, care has to be taken to identify experiments with relevant mixture quality and geometry in size and complexity of the compartment arrangement as well as relevant position and timing of the ignitions.

Also calculations of pressure time histories with CFD codes for a desired geometry and an appropriate scenario can be used for containment structure analyses to determine up to which frequency the DLF for the considered pressure load function increases or stays constant. The used mesh size has to be small enough to resolve all relevant pressure waves.

It has to be taken care of avoiding a disturbance in the recorded or calculated data due to instability of the measuring system or instability of the CFD code solver, which can lead to wrong determination of the upper relevant frequency.

Waves with a frequency above the bounding frequency of the structure have no significant effect on the structure response since their contribution is negligible due to high frequencies.

The adequate determination of the pressure load function depends on the mesh size required for the calculation, and the knowledge of upper limits of the relevant frequencies of the pressure wave that can be relevant for the structure response.

This can be determined from structural analysis as mentioned in the previous Section 2.1 if an accurate and relevant pressure load function is available.

The accuracy of the calculated pressure wave associated with its frequency depends on the mesh size. Thus the following treatment has to be done to check, if the mesh size was small enough for obtaining an accurate calculated pressure wave resolved up to the upper limit of the relevant frequency for the structure response.

For clarification a one-dimensional pressure wave propagation is treated here (as it occurs in a piping system). The potential extension into other dimensions is obvious.

Schematically Fig. 2 shows a wave with a wavelength of Λ.

The pressure wave can be well resolved with 9 points and still acceptable with 5 points for a given frequency of the wave.

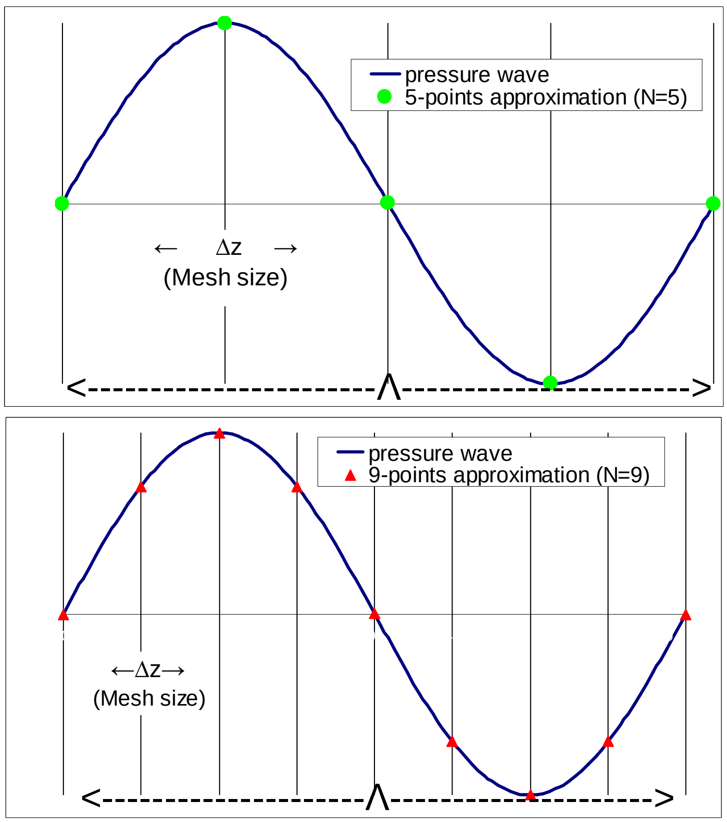

Fig. 2: 5-point approximation of the pressure wave (upper panel) and 9-point approximation of the pressure wave (lower panel).

The wavelength Λ is given by

$$\Lambda = \frac{C}{f}, \tag{13}$$

where

C: speed of sound in the gas mixture,
f: frequency of the wave.

The required mesh size Δz can be calculated from:

- the maximum relevant frequency f of the structure response
    - structure characteristic (result of structural analysis),
- the minimum speed of sound C expected in the gas mixture
    - mixture characteristic (result of calculation),
- and the required accuracy
    - number of points N (user choice):

$$\Delta z = \frac{C}{N\, f}\,. \tag{14}$$

The smallest mesh size occurs for pure air and low temperature in the containment, since the speed of sound in a gas mixture of air/steam/H_2 increases with increasing of the volume concentration of hydrogen and/or steam and with the square root of temperature (see Fig. 4).

To identify the maximum mesh size $\Delta z^{\max}$ for a conservative determination of the containment structure response the following points have to be taken into account:

Temperature

- take the lowest gas mixture temperature $T_{gas}^{\min}$ in the confinement.

Frequency

- determine the highest relevant frequency $f_{relevant}^{\max}$ from an assessment of $DLF^{\max}\left(f_k\right)$ of considered load.

Number of points

- use the minimum sufficient number of points $N_{sufficient}^{\min}$ for an accurate approximation of the pressure wave.

$\Delta z_{mesh\,size}^{\max}$ can be written as follows:

$$\Delta z_{mesh\,size}^{\max} = \frac{C_{dry\,air}^{\min}\left(T_{gas}^{\min}\right)}{N_{sufficient}^{\min}\;\; f_{relevant}^{\max}}\,. \tag{15}$$

In case the number of points is just sufficient for an approximation of the wave with the maximum relevant frequency $f_{relevant}^{\max}$, all waves with a lower frequency are determined with a higher accuracy. Thus the lower the frequency is, the higher is the accuracy of the resolution of the wave for the same number of points (see column 2 in Table 1).

Since the influence of the higher frequencies is weaker in comparison with the lower frequency, a five point approximation of the pressure wave with the limit frequency is sufficient and accurate enough for the calculation of the containment response.

3. COMBUSTION ANALYSIS FOR THE EPR™ CONTAINMENT

The method described above is used to verify the applied mesh size for the combustion calculation with the CFD code COM3D (Kotchourko et al. 1999). In fact for the determination of the mesh size a conservative pressure load function from relevant combustion experiments should be used. Unfortunately such an experiment in a large confinement is beyond practicability.

To assess the difference between the mesh size used in COM3D calculations and the appropriate upper limit for reliable analyses of containment response, the EPR™ combustion calculation for a particular scenario with the highest flame velocity has been chosen as a conservative case (Eyink et al. 2001).

The COM3D combustion calculation was based on the gas distribution calculation with the GASFLOW code (Travis et al. 1998). Fig. 3 (left panels) shows for this scenario the pressure time history at three different locations in the containment.

These pressure load functions have been used for the determination of $DLF^{\max}(f_k)$ associated with the containment response. The results can be seen in Fig. 3 (right panels).

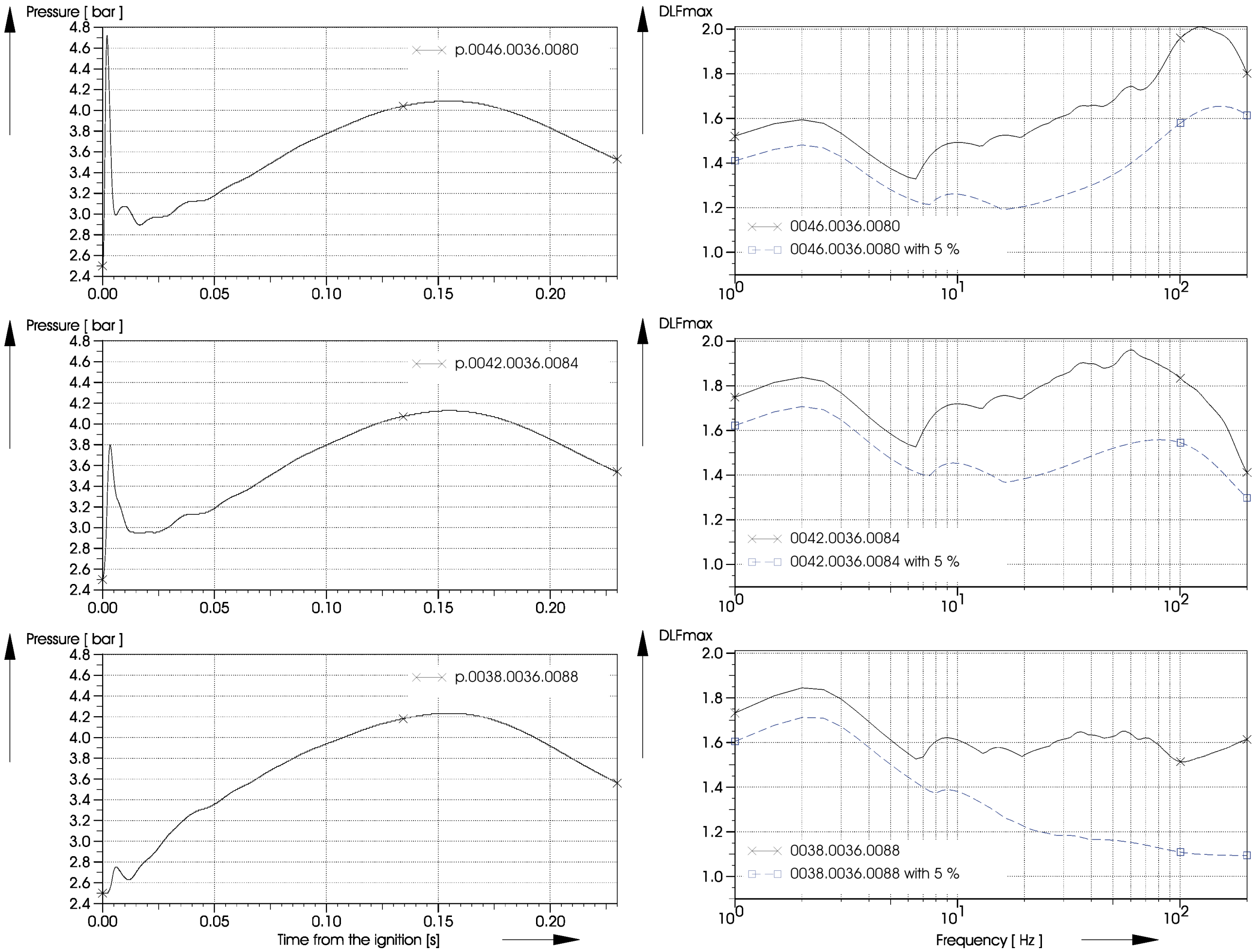

Fig. 3: Pressure histories from a combustion calculation with COM3D (left panels) and calculated maximum DLFs from the pressure load functions without and with 5 % damping (right panels).

All three DLF^{max} with or without damping decrease for frequency higher then 150 Hz, 60 Hz and 3 Hz in the upper, middle and lower panel of Fig. 3 (right side) respectively. For the considered loads the relevant frequency can be at most 150 Hz, which limits the mesh size depending on mixture quality and temperature (Table 1).

The speed of sound for the determination of the maximum mesh size is shown in Fig. 4. It is plotted for different steam volume concentrations and two temperatures, 300 K and 500 K, against the hydrogen volume concentration.

The calculated maximum mesh size $\Delta z_{mesh\,size}^{max}$ for a 9-point pressure wave approximation against the natural frequency up to 500 Hz can be seen for two mixtures, namely dry air and pure hydrogen, at 300 K in Fig. 5. For all other mixture qualities including steam, the mesh size for the same temperature lies always between these two lines (here in a logarithmic scale).

As explained above, natural frequencies above 200 Hz are not relevant for containment structural analyses.

Since the speed of sound is proportional to the square root of temperature, the maximum mesh size can be normalized with $\sqrt{T}$. Fig. 6 shows the result of the normalized maximum mesh size against the maximum relevant frequency for the containment response and a 9-point approximation of the wave. With this graph the maximum mesh size can be easily determined for all relevant temperatures.

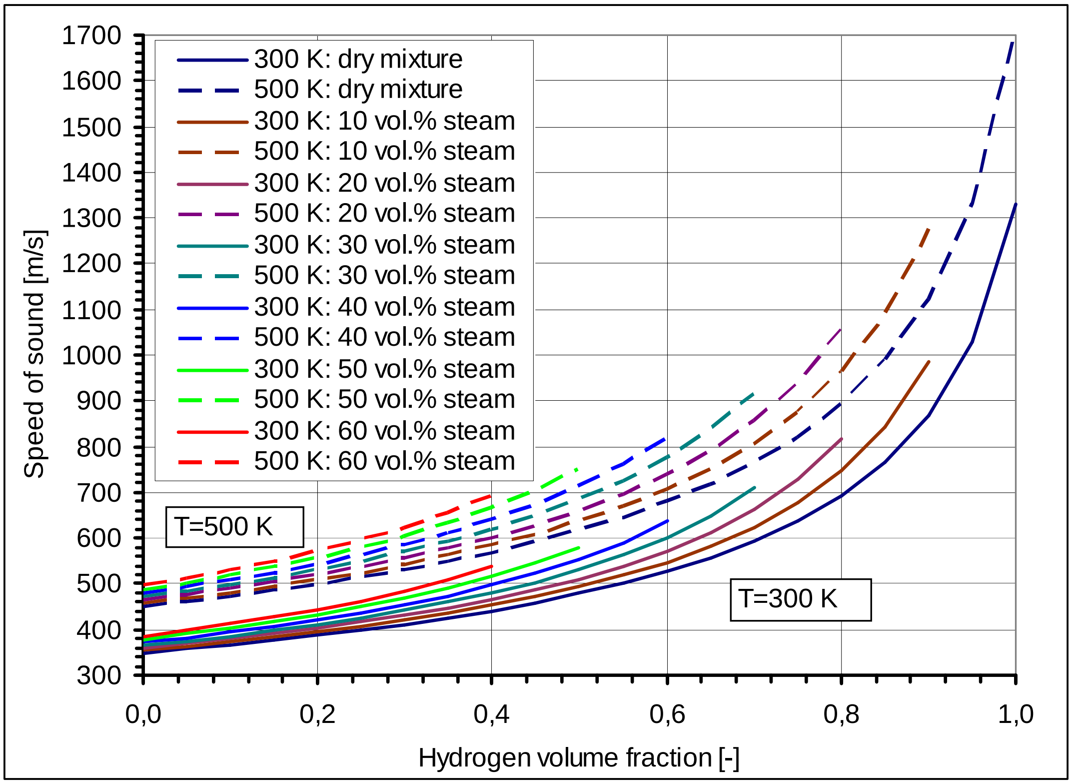

Fig. 4: Speed of sound in air/hydrogen/steam against H_2 concentration for different steam volume concentration at T=300 and 500 K.

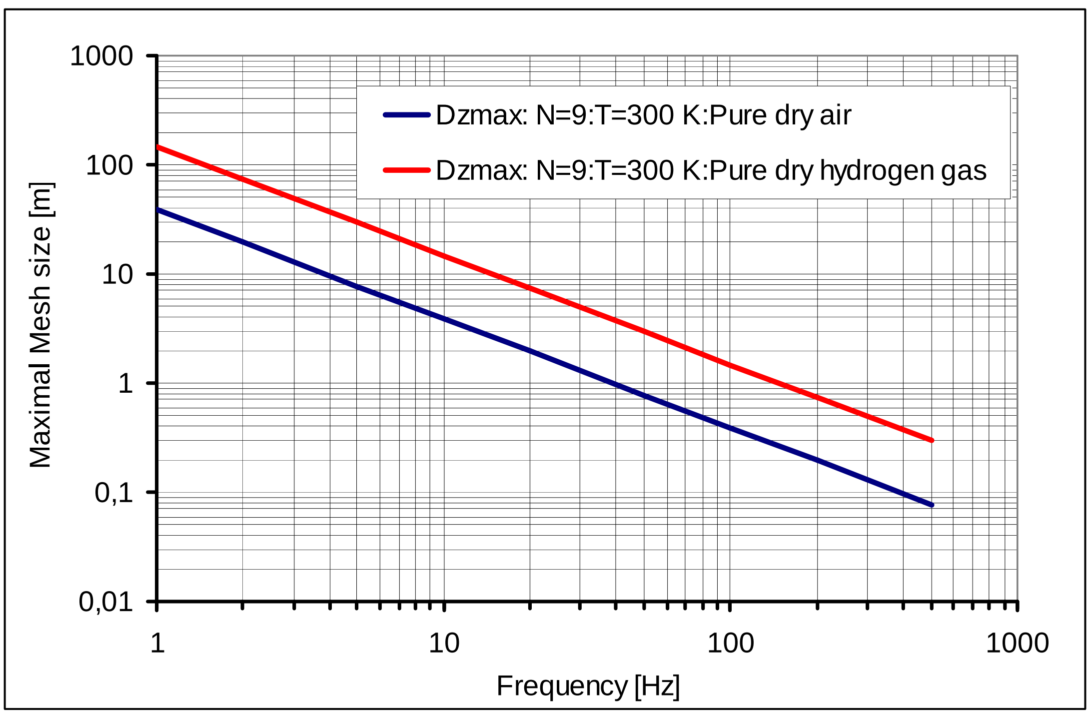

Fig. 5: Maximum mesh size against frequency for a 9-point wave approximation in dry air and pure H2 at T = 300 K

Finally, for a given natural frequency up to 500 Hz the maximum mesh size $\Delta z^{max}_{mesh\,size}$ can be extracted from Fig. 7 for a given temperature T and number of points N intended to be used for the pressure wave characterization.

If the relevant frequency is known from the DLF^{max} frequency history in Fig. 3 (right panels), for the desired temperature and number of points for the approximation of the pressure wave the maximum mesh size can be extracted for dry air and pure hydrogen from Fig. 7. For all other mixture qualities (air/steam/H_2) the maximum mesh size can be determined using the relation for calculating $\Delta z^{max}_{mesh\,size}$ (Eq. 15) and Fig. 4 for calculating the speed of sound of the corresponding mixture quality for a given appropriate number of points.

The maximum mesh sizes calculated for different relevant frequencies for the structure response and mixture quality are listed in Table 1.

Table 1: Maximum mesh sizes for different relevant natural frequencies and some other parameters

$f^{max}_{relevantt}$	$N^{min}_{sufficient}(f^{max})$ $N^{min}_{appropriate}(f_{lower})$	$T^{min}_{at\,initiation\,of\,combustion}$	$v^{min}_{hydrogen}$	v^{min}_{steam}	$C(v^{min}_{steam}, v^{min}_{hydrogen}, T^{min}_{mixture})$	$\Delta z^{max}_{mesh\,size}$
[Hz]	[-]	[K]	[vol %]	[vol %]	[m/s]	[m]
50	5 ($f^{max}_{relevant}$ = 50 Hz)	300	0	0	349	1.39
	10 (25 Hz)			20	359	1.44
	25 (10 Hz)		10	0	366	1.47
				20	379	1.52
		500	0	0	450	1.80
				20	464	1.85
			10	0	473	1.89
				20	489	1.96
100	5 ($f^{max}_{relevant}$ = 100 Hz)	300	0	0	349	0.70
	10 (50 Hz)			20	359	0.72
	20 (25 Hz)		10	0	366	0.73
	25 (20 Hz)			20	379	0.76
	50 (10 Hz)	500	0	0	450	0.90
				20	464	0.93
			10	0	473	0.95
				20	489	0.98
200	5 ($f^{max}_{relevant}$ = 200 Hz)	300	0	0	349	0.35
	10 (100 Hz)			20	359	0.36
	20 (50 Hz)		10	0	366	0.37
	40 (25 Hz)			20	379	0.38
	50 (20 Hz)	500	0	0	450	0.45
	100 (10 Hz)			20	464	0.46
			10	0	473	0.47
				20	489	0.49

The green numbers in the second column indicate the corresponding number of points for the resolution of the lower frequency (in parenthesis) of the pressure wave, which increase with decreasing frequency.

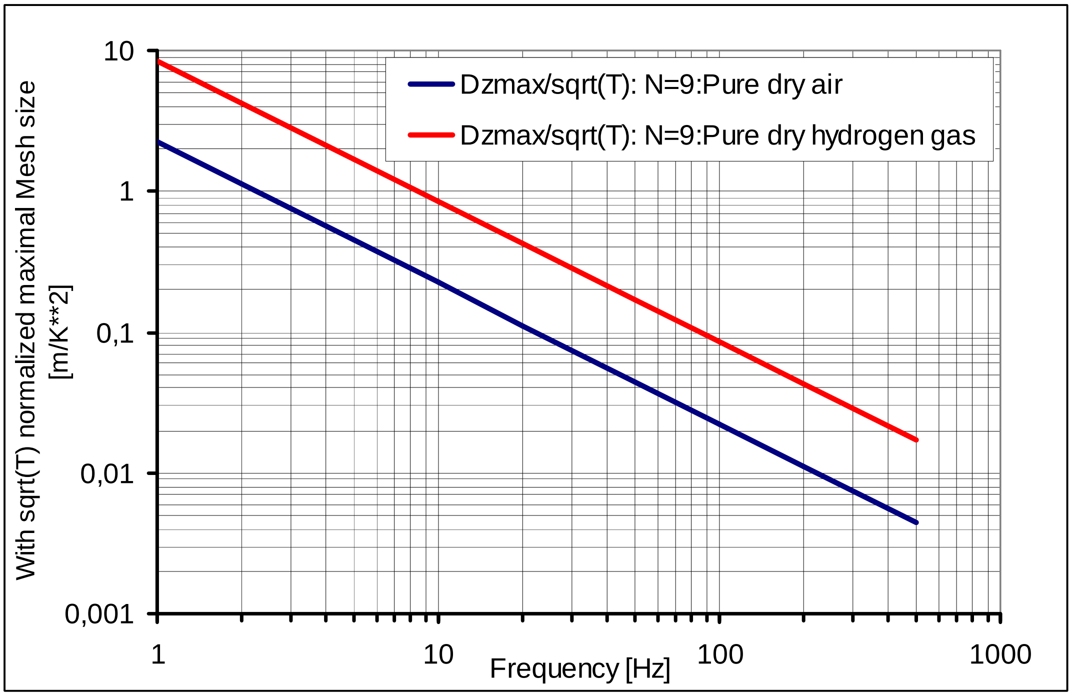

Fig. 6: Maximum mesh size normalized with $\sqrt{T}$ against frequency for a 9-point wave approximation in dry air and pure H_2

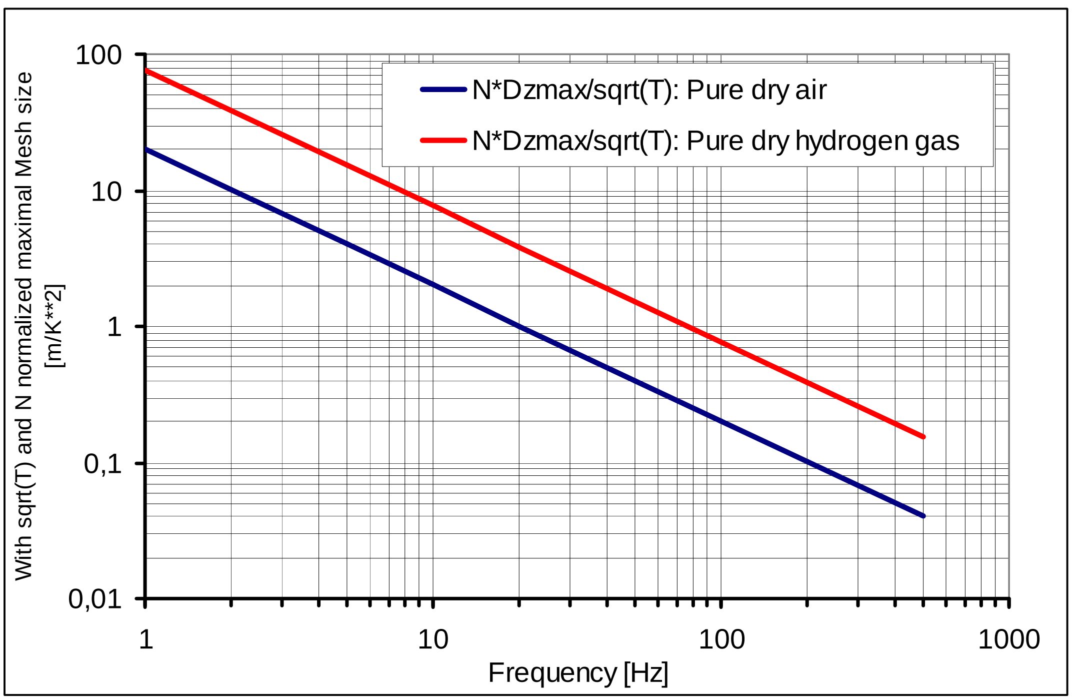

Fig. 7: Maximum mesh size normalized with $\sqrt{T}$ and N against frequency in dry air and pure H_2

The maximum calculated mesh size is between 2 m and 0.4 m for a frequency between 50 and 200 Hz, a temperature between 300 and 500 K, a hydrogen concentration between 0 and 10 vol% and a steam concentration between 0 and 20 vol%, respectively. The choice of a 0.4 m mesh size for the COM3D

EPR™ combustion calculation is apparently small enough to resolve at least waves up to 200 Hz with acceptable accuracy.

It should be mentioned that the above methodology could be applied also to the response of a piping system to pressure wave propagation.

4. CONCLUSION

This theoretical treatment shows that the maximum mesh size for a combustion calculation

- depends on the highest relevant natural frequency of the structure,
- depends on the required accuracy for the pressure wave approximation
    - 9 points is good enough
    - up to 5 points is acceptable for the maximum relevant frequency and is good enough for the lower frequency,
- decreases with increasing relevant natural frequency of the structure,
- increases with increasing gas temperature,
- increases with increasing H_2 and/or steam concentration.

For EPR™ containment pressure load analyses the maximum relevant natural frequency of the outer structure is lower than 150 Hz, which leads to a maximum mesh size of about 60 cm.

Furthermore, it has to be investigated whether a higher natural frequency of the structure for other pressure load function resulting from other scenarios is relevant.

The EPR™ COM3D calculations are acceptable because of their small mesh size of 40 cm. This size is small enough to resolve all pressure waves, which are relevant for the containment structure response.

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