Numerical Modelling of Detonation Performance

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Detonation performance is defined in terms of the steady state wave structure of the detonation front, and the initiation behaviour of the explosive. Some common techniques for modelling detonation performance are described, based on semi-analytic hydrodynamic and computational fluid dynamic reactive flow models. Accurate modelling of detonation performance is shown to require resolution of the reaction zone in the explosive, for non-ideal and for intrinsically unreactive systems. The ability of detonation models to predict steady state and initiation performance is discussed. Examples of resolve reaction zone models of explosives of varying degrees of ideality are presented. The sensitivity of predictions to primary data is examined for steady state reaction zone modelling of the insensitive explosive PBX W115, and Composition B3. Future directions for development of reactive flow models are examined. Particular emphasis is drawn to the need for more detailed temperature dependent kinetic schemes, and the inclusion of more detailed reaction geometries in such flow models.

1. Introduction

The use of interpretive and predictive models has been an important tool in obtaining a conceptual and quantitative understanding of detonation phenomena (Mader 1979; Fickett & Davis 1978). Modelling also has been important in understanding the utilization of energy released by detonation in performing useful work on surrounding material (Wilkins 1964).

Recently, significant theoretical developments have occurred in the various physical sciences associated with detonics: equations of state of condensed matter, reaction kinetics, and computational fluid dynamics. These have extended the accuracy of detailed numerical simulations of detonation, to an extent that performance predictions based on modelling have become a useful and reliable tool.

In this work, a hierarchy of detonation models is described and examples given of some recent results on performance predictions for various conventional and non-ideal explosive systems. The limitations of current computational approaches are assessed and future directions sought.

2. Modelling technique

Elements of detonation performance modelling include the behaviour of the explosive, the material in which the explosive detonates and the target material against which the explosive works. These factors can be classed as either intrinsic to the explosive or imposed upon the explosive by its surroundings. Although it is not

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possible to derive performance parameters based solely on intrinsic properties, the advent of general purpose computer codes for solving problems involving shock hydrodynamics in multi-material systems (Wilkins 1964; Mader 1979; Hallquist 1976), has reduced the kernel of modelling detonation performance to that of representation of the detonation process within such codes.

Detonation models are required to reproduce two intrinsic performance criteria, the physical structure of the detonation wave, and the propensity of the detonation wave to initiate or fail. Various approaches may be used to accomplish these ends, resulting in differing degrees of refinement in the final solution.

The minimum required level of refinement can be estimated from the ratio of the time for chemical reaction in the explosive to the characteristic response time of the target. If the target response is sufficiently long, a simple model of detonation may be used. However, if reaction times are close to the response time of the target, complete resolution of the reaction zone in the explosive may be required. The highly nonlinear nature of initiation and failure precludes the use of simple models, and a detailed reactive flow model must be used if the performance of the system is to be correctly represented (Leiper & Kennedy 1989*b*).

Numerical models of detonation in condensed matter normally are based on solutions of the Euler equations for invicid, irrotational, compressible flow with source terms for chemical reaction (Fickett & Davis 1979)

$$\dot{\rho}+\rho \operatorname{div} \boldsymbol{u}=0, \quad \dot{\rho}\boldsymbol{u}+\operatorname{grad} p=0, \quad \dot{E}+p\dot{v}=0, \quad \dot{\beta}=\boldsymbol{r},$$

where ρ is density, $\boldsymbol{u}$ particle velocity, p pressure, E internal energy, v specific volume, β the fraction of total heat release, and $\boldsymbol{r}$ the chemical reaction rate vector.

Closure requires the addition of chemical reaction rate equations, and an equation of state describing the locus of thermodynamic state variables available to the system, as a function of the extensive thermodynamic variables and the composition of the reacting material. If the response of the explosive to shock loading is other than that of a simple fluid, a constitutive model must be included also.

3. A modelling hierarchy

By use of simplifying assumptions, various levels of model can be developed from the field and closure equations. These may be ordered into a hierarchical approach to modelling detonation performance, ranging from simple models of the structure of a steady state detonation wave, through to the simulation of evolutionary processes in arbitrary geometry. A logical approach is proposed consisting of ideal detonation, non-ideal semi-analytic wave, and computational fluid dynamic models.

The first level, and the most radical assumption, is that of ideal detonation. Chemical conversion is assumed to occur infinitely quickly, with chemical, mechanical and thermal equilibrium between all reaction products. The Chapman–Jouguet (CJ) hypothesis is invoked to give a single solution to the equations of motion which characterizes the maximum velocity at which a detonation wave can propagate stably in the explosive. Total available energy, calculated by some arbitrary release path from the sonic (CJ) point can also be evaluated. Accurate computation of the ideal detonation state requires only that the equilibrium equation of state of the reaction products be accurately computed. Under the assumption of ideal detonation, the performance is assessed on the basis of the CJ pressure or detonation velocity, and the calculated available energy.

An extension of this model to dynamic simulations in arbitrary geometry is possible, by use of Huygens constructions, in which an ideal CJ wave is propagated through the explosive in a predetermined manner (Wilkins 1964). Neither the reaction zone, nor the dynamic wave properties are modelled in this process.

The next level of sophistication comes from inclusion of a chemical reaction rate vector, giving reactive flow models. Steady state wave arguments can be invoked, enabling the wave structure to be found semi-analytically, leading to the Zeldovich–von Neumann–Doring (ZND) model (von Neumann 1962) in one space dimension. Addition of terms for flow divergence extends ZND theory to axisymmetric geometry, modelling charge diameter effects and reactivity effects (Wood & Kirkwood 1954; Chan 1981; Kirby & Leiper 1985; Bdzil 1981). The result of confinement can be modelled, providing the effect on the hydrodynamic flow field can be included in the solution.

For time-dependent problems, spatial and temporal discretization schemes are used to integrate the partial differential equation system with appropriate closure models and initial conditions (Mader 1979; Lee & Tarver 1980).

4. The chemical reaction rate vector

The functional form chosen for the chemical reaction rate vector is the central factor in determining the success of resolved reaction zone models. Reaction rate vectors for condensed explosives have sought to decouple the effect of intrinsic chemical reactivity from that of reaction geometry, thus modelling the heterogeneous nature of composite explosives, and the inherently heterogeneous temperature field created in such systems by shock compression. The underlying primary chemical reactions are neglected, in favour of a lumped parameter representation of the molecular reaction scheme.

The progenitor of such work was the Ignition and Growth model (Lee & Tarver 1980)

$$\dot{\beta} = I(1-\beta)^x (v_o/v_e)^r + G(1-\beta)^x \beta^y p^z,$$

where v was specific volume, subscripts o, e referred to the porous unshocked and dense shocked states respectively, and I, G, r, x, y, z were fitting factors. A generalization to multi-phase multi-component mixtures, was proposed by Kirby & Leiper (1985):

$$\dot{\beta} = (1-\beta)\left\{\frac{a_h(p-p_h)^{b_h}}{t_h} + \frac{a_1 p^{b_l}}{t_l} + \frac{a_s p^{b_s}}{t_s}\right\},$$

where the subscript h, l, s referred to hot-spot, matrix and included solid phases within the explosive. The a_i (i = h, l, s) were form functions, dependent only on the initial formulation and degree of reaction of the explosive, which were used to model the reaction geometry. This function is used for the examples given below.

Traditionally, pressure has been used as the thermodynamic variable in the chemical reaction rate. Some workers, notably Chan (1981), and Johnson *et al.* (1985), have used mixed pressure and temperature dependent laws to describe the shock initiation event. Johnson *et al.* have been particularly successful in modelling the changes in shock initiation behaviour with changing density, and in modelling dynamic desensitization by precursor shocks. The added complexity of solution of the temperature field in addition to the hydrodynamic flow generated a large computational overhead.

Table 1. *Composition of explosives*

Composition B3	RDX 63 %	TNT 37 %		
RDX emulsion[a]	RDX 35 %	NH_4NO_3 51 %	H_2O 10 %	oils 4 %
PBX W115	RDX 20 %	NH_4ClO_4 45 %	Al 25 %	HTPB 12 %
Polar Saxonite[b]	NG ≈ 25 %	NH_4NO_3 ≈ 50 %		

[a] Manufactured with either fine ($592.5\ m^2\ kg^{-1}$) or coarse ($55.6\ m^2\ kg^{-1}$) RDX.

[b] Proprietary formulation, exact composition not available.

5. Application to steady state detonation

An analytic wave theory was used to model the detonation performance of a conventional high explosive, and three novel systems. The explosives ranged from a mixture of monomolecular explosives (Composition B3), to composite systems comprising admixtures of a sensitizing mono-molecular explosive and energising phases of oxidisers and fuels (see table 1). The intimacy of mixing of the energising phases was varied over the range 10^{-7} m, in cyclotrimethylene trinitramine (RDX) sensitized emulsion, to 10^{-5} m in PBX W115.

Initially an ideal detonation state calculation was performed. A non-ideal detonation model was then used to modify the ideal performance, to account for the reactivity of the explosive, and hydrodynamic losses associated with finite charge diameter.

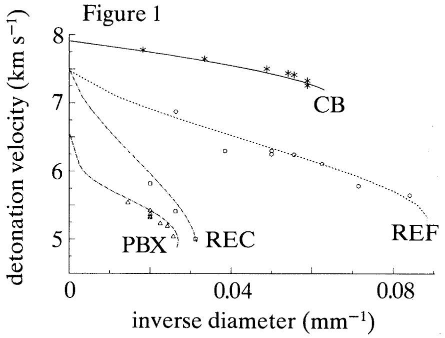
The ideal calculation was based on an intermolecular equation of state (Braithwaite & Byers Brown 1989) (see table 2). From the calculated CJ values, and exothermicity, a clear ranking of the explosives was not apparent. A semi-analytic reactive flow analysis was therefore performed, based on a development of Wood–Kirkwood theory (Chan 1981; Kirby & Leiper 1985).

The measured detonation performance, as characterized by the charge diameter effect was used to construct a non-ideal model, as outlined in Leiper & Cooper (1989). The equation of state of the unreacted explosive, taken to be a polytropic equation of state, was calibrated to the shock compressed state on the mixture Hugoniot (Afanasenkov *et al.* 1969; Kirby & Leiper 1985). The reacted equation of state, of polytropic form with density dependent polytropic index, was fitted to an isentrope through the ideal CJ point as calculated above. A simple mixing law based on the local reaction coordinate was used to establish an overall equation of state of the reacting material.

The non-ideal model was calibrated by fitting the slightly divergent flow theory to the measured charge diameter effect data (Malin *et al.* 1957; Leiper & Cooper 1989; Forbes *et al.* 1989), using the kinetic rate constants as unknowns (see figure 1). The resultant model was used to predict the variation of wave structure with charge diameter.

An *ad hoc* quantitative measure of performance was adopted for ease of presentation of the results. The CJ distance and degree of chemical conversion were chosen for this purpose: the CJ distance described the natural length scale of the process, and the degree of chemical conversion the deviation from ideality in the system. By studying these two parameters the overall performance of the explosive in any application could be assessed.

Composition B3 was found to be the most ideal system in terms of degree of chemical conversion at the CJ plane (see figure 3). This was as expected. Surprisingly, the RDX sensitized emulsions were found to be more ideal than PBX W115,



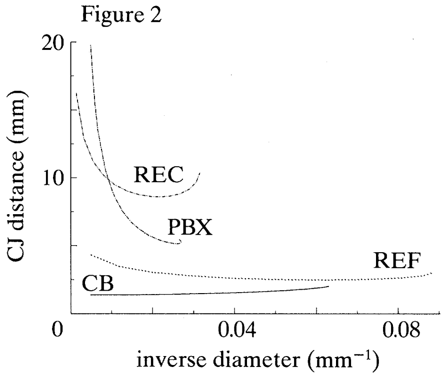


Figure 1. Variation of detonation velocity with inverse charge diameter for composition B3 (CB), emulsion sensitized with fine RDX (REF), emulsion sensitized with coarse RDX (REC), and PBX W115 (PBX). Solid lines were from the model, discrete points were from experiment. Note that the CB diameter is scaled by ×5.

Figure 2. Variation of reaction zone length with inverse charge diameter. Labels as figure 1. Note that the CB diameter is scaled by ×5 and the CJ distance is scaled by ×10.

Table 2. *Ideal Chapman–Jouguet values*

	detonation velocity (km s^{-1})	heat of reaction (MJ kg^{-1})	CJ adiabatic exponent
Comp. B3	7.911	5.692	3.240
RDX emulsion	7.470	3.90	3.240
PBX W115	6.535	8.20	1.642
Polar Saxonite	5.902	3.211	3.571

notwithstanding the greater velocity decrement at failure for the emulsion systems. The effect of morphology on ideality was evident in the RDX sensitized emulsion, with finer RDX particles giving a more ideal system: presumably by reduction in the web thickness between initiation sites in the explosive. This again was as expected, and has been further analysed by Leiper & Cooper (1990).

The extremely low reactivity of PBX W115 was worthy of comment, given that the velocity decrement at failure was less than 25% of the ideal value. Experimental evidence on the reactivity of a similar composition (Bai & Ding 1989) was in good agreement with the degree of conversion found here.

Further evidence of the relative performance of these systems was found in the reaction zone length predictions (see figure 3). The variation of reaction zone length did not rank simply with non-ideality, but reflected the intrinsic reactivity of the explosives. The reaction zone length of the non-ideal systems were found to increase with increasing diameter, characteristic of partial reaction at the sonic plane. Moreover, the variation was not monotonic nor order preserving, in that the reaction zone of PBX W115 varied from below, to above, that of the coarse RDX sensitized emulsion, although the degree of reaction of PBX W115 was always much less than that of the emulsion.

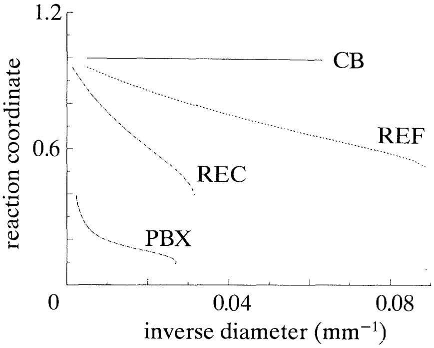


Figure 3. Variation of CJ degree of reaction with inverse charge diameter. Labels as figure 1. Note that the CB diameter is scaled by ×5.

6. Application to unstable systems

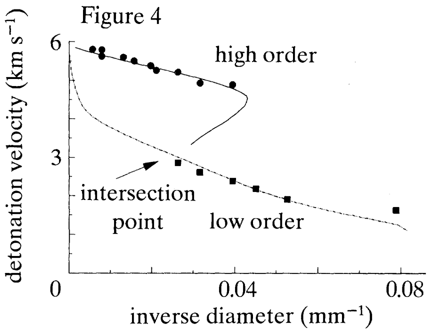
The problem of catastrophic variation of detonation performance between two stable states has been recorded for several explosives (Taylor 1952; Hino & Hasegawa 1959). A conceptual understanding of the phenomenon, based on a switch from grain burning reaction to mass thermal explosion was postulated by Taylor (1952). A theoretical assessment based on reactive flow modelling was presented by Leiper & Cooper (1989). In this work, semi-analytic non-ideal detonation modelling was applied to an explosive displaying such catastrophic behaviour, to elucidate the consequence of such instability on detonation performance.

The experimental diameter effect of Polar Saxonite (table 1, figure 4) (Paterson 1948), displayed two stable solutions, high and low order. An ideal calculation (table 2) agreed well with the asymptote of the high velocity régime. A non-ideal model of the system was therefore pursued, based on the measured diameter effect curve and the predicted ideal state.

Initially one parametrization of the chemical rate equation was sought that would reproduce both high and low velocity régimes, however, the form of the rate equation used in the model was unable to fit both régimes simultaneously. The charge diameter curve therefore was modelled in separate parts, corresponding to the high and low velocity régimes. Two solutions were found, one reproducing the low-order data, the other reproducing the high-order data (figure 4). The kinetics required to reproduce these were hot spot and grain burning for low order, and abrupt thermal explosion for high order.

The effect of the discontinuity on performance was marked, the low velocity régime having an extended reaction zone and much lower degree of reaction at the sonic plane (see table 3).

The existence of discontinuities in the diameter effect curve had previously been described (Leiper & Cooper 1989) in terms of two stable solutions: a conventional high-order solution, in which all velocities were allowed, and a low-order solution in which the only allowed velocities were between the intersection of the lower branch of the high-order solution with the upper branch of the low-order solution, and the low-order critical diameter. Data from this study was in agreement with this hypothesis (see figure 4).



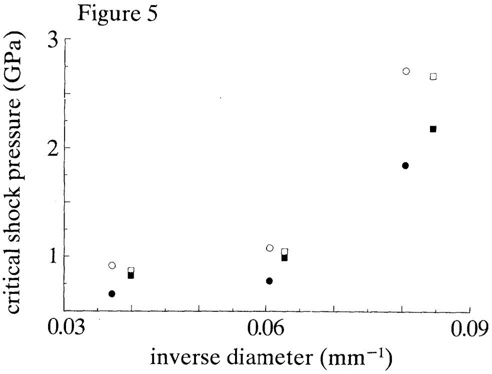


Figure 4. Variation of detonation velocity with inverse diameter for high and low order behaviour of Polar Saxonite. Solid lines were from the model, discrete points were from experiment.

Figure 5. Variation of critical initiation pressure with inverse charge diameter. ●, Predicted fail; ○, predicated pass; ■, experimental fail; □, experimental pass.

Table 3. *Low and high velocity performance measures*
(All lengths in millimetres)

charge diameter	CJ distance		CJ degree of reaction	
	low order	high order	low order	high order
25	10.57	4.45	0.022	0.71
43	14.34	4.10	0.054	0.82

7. Application to time-dependent systems

The modelling of shock initiation, wave collision, and failure, requires the solution of the full time-dependent flow field, with a chemical source term that is capable of representing the reaction behaviour of the explosive over a large region in pressure–temperature hyperspace. The required performance predictions are those of the criticality conditions for initiation or failure, and the structure of the wave as it approaches steady-state behaviour.

Many workers have been active in this field. As an example of typical calculations, the work of Leiper & Kennedy (1989*a*) is reproduced below.

A semi-analytic non-ideal model was used to calibrate a reactive flow kinetic rate equation from measured diameter effect data. The calibration was then used in a finite element hydrocode to predict the effect of charge diameter on the critical initiation pressure in a large-scale gap test, the subject of experimental studies by Leiper & Cooper (1987). The predicted results were in good agreement with experiment (see figure 5).

8. Sensitivity to initial data

An assessment of the growth of errors in the proposed modelling chain was carried out. The effect of inaccuracies in the source data on the calibration of reactive flow models was examined. In particular the sensitivity of the calculation to errors in the unreacted and reacted equations of state was evaluated.

Figure 6

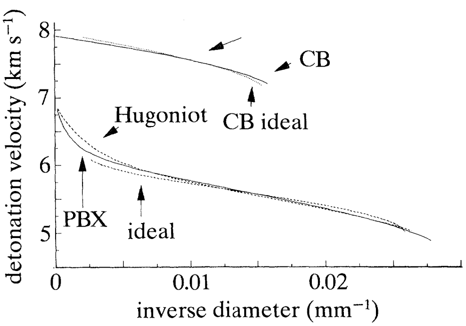


Figure 7

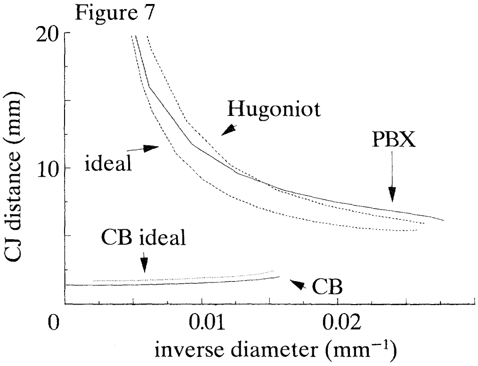


Figure 6. Variation of detonation velocity with inverse charge diameter for Composition B3, and PBX W115 for various initial data. Line labels are given in table 4. Note that the diameter of CB and CB ideal are scaled by ×5.

Figure 7. Variation of reaction zone length with inverse charge diameter. Labels as figure 6. Note that the diameter of CB and CB ideal are scaled by ×5, and the CJ distance is scaled by ×10.

Table 4. *Values used in error analyses*

	detonation velocity ($\mathrm{km\ s^{-1}}$)	heat of reaction ($\mathrm{MJ\ kg^{-1}}$)	CJ adiabatic exponent	Hugoniot A ($\mathrm{km\ s^{-1}}$)	Hugoniot B ($\mathrm{km\ s^{-1}}$)	data label
PBX W115	6.978	8.20	3.195	3.0	1.45	PBX
	6.978	8.20	3.195	2.46	1.60	Hugoniot
	6.535	8.20	1.649	2.46	1.60	PBX ideal
Comp. B3	7.911	5.692	3.240	3.01	1.40	CB
	7.979	5.602	2.471	3.01	1.40	CB ideal

Composition B3 and PBX W115 were chosen and small changes made to the equations of state parameters. The changes reflected the different results obtained in calculating the unreacted mixture Hugoniot from different source data, and in performing ideal state computations using JCZ (Cowperthwaite & Zwisler 1976), and IDeX (Braithwaite & Byers Brown 1989) equations of state (see table 4). For each change in the initial data, a best fit to the experimental performance data was recomputed using the kinetic rate parameters as independent variables.

Significant differences in ideal code prediction and Hugoniot calculations were found for PBX W115. The reactive flow model was shown to be sensitive to the unreacted and reacted equation of state parameters, although equally good fits to the experimental data could be obtained in all cases (see figure 6). Qualitatively, the results of the analyses were very similar. The type of kinetic function required to fit the data, hot spot and grain burning, did not alter, although a scaling of the absolute rate was required to reproduce the experimental data. Quantitative measurements of detonation performance, based on the differing kinetic parameters, displayed some variation (figures 7 and 8) with changes to the reaction zone length, and CJ reaction coordinates of the order of 20% in certain regions of the diameter effect curve. The sensitivity to the various effects was such that compensating errors could occur (figure 8 curves PBX and ideal). Differences in ideal code predictions for Composition

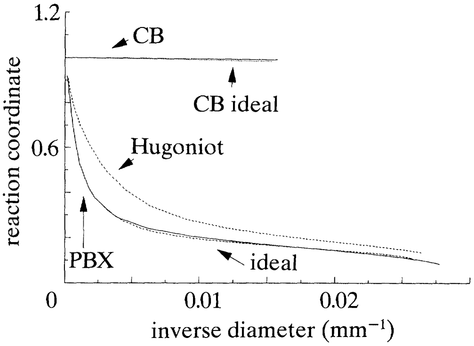


Figure 8. Variation of CJ degree of reaction with inverse charge diameter. Labels as figure 6. Note that the diameter of CB and CB ideal are scaled by × 5.

B3 were found to be small. Some effect was noted in the calculated reaction zone length, but the qualitative and quantitative variation in performance was not significant.

9. Areas for future research

Significant progress has been made in modelling detonation performance of explosives. However, many areas of reactive flow modelling remain ill-defined, and limit the ability of such models to provide a predictive capability.

Much of the problem is at present hidden by the common practice of parameterizing chemical reaction rate equations in reactive flow models, by using the models themselves to reduce experimental data. This procedure provides a self-consistent solution for the calibration data, but does not guarantee the absence of compensating errors. A more detailed kinetic scheme, capable of independent calibration should be sought to eliminate this problem. Towards this end, the effects of intrinsic reactivity and local reaction geometry must be better understood at a fundamental level to improve the reliability of reactive flow predictions. The adoption of temperature driven reaction rates in condensed phase detonation models would be a major, if computationally expensive, advance.

The error analysis carried out above, underlined the requirement for development of suitable equations of state for partly and fully reacted explosive. Increased confidence in defining ideal CJ state parameters from which reactive flow models derive source data would greatly increase the confidence of onward prediction. The topic of mixture theories for equations of state of reacting flows has not been well investigated, but such models will be required to improve reaction zone structure predictions.

10. Conclusion

Various aspects of numerical modelling of detonation performance have been discussed. An overview of the concept of detonation performance, and the levels of models that can be used to represent the performance of explosive systems has been presented. Accurate representation of the detonation wave structure has been emphasised as the singularly most important facet of any detonation performance model for use with non-ideal explosives.

A detailed account has been given of the basis of most numerical models of detonation. Strengths and weaknesses of some have been enumerated. Examples have been given of results from one resolved reaction zone model. For two resolved reaction zone studies, some indication has been given of the effect of uncertainties in key source data on the model prediction.

Finally a view was presented on areas of greatest uncertainty in resolved reaction zone calculations for use in detonation performance assessments.

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