Fracture Mechanics of Concrete Structures
Proceedings FRAMCOS-3
AEDIFICATIO Publishers, D-79104 Freiburg, Germany

OPTIMUM DESIGN OF PLAIN AND FIBRE-REINFORCED CONCRETE MIXES BASED ON FRACTURE MECHANICS

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Abstract
The characteristic length l_{ch} is used as a brittleness measure for the design of plain and fibre-reinforced concretes by applying the methods of mathematical optimization. Micromechanical relations for the elastic modulus E, specific fracture energy G_F, tensile strength f_t' and compressive strength f_c' are provided and the nonlinear mathematical problem of the maximization of $l_{ch} = EG_F/f_t'^2$ is solved subject to an equality constraint on f_c'. In this way optimal values for the microstructural parameters (e.g. water/cement ratio, aggregate size, length of fibre and volume fractions of aggregate and fibre) are obtained.
Key words: Brittleness, optimization, fracture mechanics, characteristic length, mix design, DSP

1 Introduction

There is growing recognition in the structural design and research community of the fact that the implementation of a material/structural brittleness measure in the design of plain and reinforced concrete can improve structural reliability by providing uniform safety margins over a wide range of structural sizes and material compositions. The safety margin typically depends on the accuracy of the prediction of a structure's load-bearing capacity and on the assumptions made regarding the material properties, applicable analysis method and the structural failure mode. Notwithstanding this knowledge, the current practice of design generally ignores the fact that the accuracy of assumptions and predictions is affected by the structural size and material composition (for a review of experimental evidence, see Lange-Kornbak (1997)).

To describe the variations in the relative load-carrying capacity (i.e. the ratio of nominal strength to direct tensile strength) and the failure mode of concrete structures/specimens with the structural/specimen size and the material composition, principles of fracture mechanics have provided various brittleness measures (see Lange-Kornbak (1997) for a review). They consistently indicate that the characteristic length introduced in the Fictitious Crack Model, Hillerborg et al. (1976), is an appropriate measure for describing the effect of the material composition, Lange-Kornbak (1997). The characteristic length is defined as $l_{ch} = EG_F/f_t'^2$ where E is the modulus of elasticity, G_F the specific fracture energy, and f_t' the direct tensile strength. As l_{ch} is the measure controlling the nominal strength and failure mode, it ought to be taken into consideration in the design of concrete mixes. However, the traditional approach to design of concrete mixes is restricted to driving only two mechanical properties, typically the compressive strength f_c' and the mix workability, to target values. This is due to the fact that this heuristic approach is unable to accommodate more than two design criteria. However, by formulating the design problem as a mathematical optimization problem, efficient search techniques and convergence criteria can be brought to bear on the solution, so that problems involving many design variables and criteria can be successfully solved. In this work it is demonstrated how plain and fibre-reinforced concrete mixes can be designed for a given compressive strength and maximum characteristic length by adapting the principles of mathematical optimization. The necessary micromechanical relations to achieve this are established by Lange-Kornbak & Karihaloo (1996) for plain concrete and by Lange-Kornbak & Karihaloo (1998) for fibre-reinforced concrete.

2 Micromechanical relations for plain concrete

The specific fracture energy is

$$G_F = \frac{(K_{Ic})^2(1-\nu^2)}{E(1-V_{agg})}\left\{\frac{1}{3}\left[\left(\frac{K_f}{\sqrt{2/\pi}K_{Ic}}\right)^3 - 1\right] - \ln\left(\frac{K_f}{\sqrt{2/\pi}K_{Ic}}\right)\right\} +$$

$$+\sqrt{\xi}K_f - K_f^2/(6\tau V_{agg}) \tag{1}$$

where ν is effective Poisson's ratio, E effective modulus of elasticity, K_{Ic} effective fracture toughness, ξ surface texture parameter of the aggregate with the dimension of length, τ shear strength of the aggregate- matrix interface and V_{agg} the total volume fraction of aggregates. $K_f = \sqrt{g}\sigma_f$, where g is maximum size (diameter) of the aggregate and σ_f the stress in uniaxial tension when frictional pull-out of the aggregates is the dominant toughening mechanism.

The direct tensile strength is given by

$$f_t' = \frac{\eta K_{Ic}^m}{\sqrt{\pi r_0}} \tag{2}$$

with K_{Ic}^m the fracture toughness of the matrix. The half-length of cracks r_o is related to the maximum dimension of the aggregate and the configuration of intrinsic microcracks caused by autogeneous deformation. Composites with limited microcracking have $r_o = g/2$, whereas in e.g. DSP mortars $r_o = 1.5g + 0.5g_{av}(V_s^{-1/3} - 1)$, where g_{av} is the average aggregate size and V_s the volume fraction of fine aggregate relative to the volume of mortar. The effective toughening ratio η is constructed by simple multiplication of the toughening ratios of the active toughening mechanisms. The most important toughening mechanisms are crack deflection, distributed interfacial cracking, bridging and trapping with the corresponding toughening ratios

$$\eta_d = \sqrt{1.0 + 0.87V} \tag{3}$$

$$\eta_i = \sqrt{\frac{1}{1 - (\pi^2/16)V(1-\nu^2)}} \tag{4}$$

$$\eta_b = \sqrt{1 + \frac{1}{\eta_t^2}\frac{(\pi/2)f_{t,a}'^2 g_{av} V(1-\sqrt{V})(1-V)}{(K_{Ic}^m)^2}\left\{1 - \frac{\pi^2}{16}(1-\nu^2)V\right\}} \tag{5}$$

$$\eta_t = \left\{1 - \frac{(1-V)\pi/4}{\ln\{[1+\cos(\pi V/2)]/[\sin(\pi V/2)]\}}\right\}^{-1}, \tag{6}$$

respectively. Here $f_{t,a}'$ is the uniaxial tensile strength of the aggregate. η_t takes the value 1 when the crack trapping mechanism is absent. For mortar, the matrix toughness K_{Ic}^m would equal that of the cement paste K_{Ic}^p and V would be V_s, whereas for concrete K_{Ic}^m would be the fracture toughness of mortar and V the volume fraction of coarse aggregate V_c. For $0.2 \leq w/c \leq 0.45$, the fracture toughness of cement paste at a maturity of 28 days may be established from

$$K_{Ic}^p = 0.6125 - 0.85\, w/c \quad \text{MPa}\sqrt{\text{m}} \tag{7}$$

The compressive strength follows from

$$f'_c = K \left\{ \frac{g}{g_s} \left[\left(\frac{1 - \lambda (g'/g)^\gamma}{V_{agg}} \right)^{1/3} - 1 \right] \right\}^{-0.16} \left(\frac{1 - V_{air}/(1 - V_{agg})}{1 + (w/c)(\rho_c/\rho_w)} \right)^2 \tag{8}$$

where $(\lambda, \gamma) = (0.39,0.22)$ or $(0.45,0.19)$ for rounded and sharp- edged angular aggregates, respectively, g' is the maximum size of the bottom 10% in the aggregate grading curve, g_s is the maximum size of the fine aggregate and K is an experimental constant depending upon g_s and other aggregate and cement parameters.

Cement paste, mortar, plain concrete and fibre-reinforced concrete can be regarded as two-phase composites with the modulus of elasticity

$$E = E_m \frac{n + \Theta + V\Theta(n-1)}{n + \Theta - V(n-1)} \tag{9}$$

where V is the volume fraction of the discrete phase, Θ is a geometry function accounting for the configuration of the discrete phase and n is the ratio of the modulus of elasticity of the discrete phase to the modulus of elasticity of the continuous phase (matrix), E_m. For cement paste ($E = E_p$), a distinction is made between water/cement ratios below and above $1.2\rho_w/\rho_c$ (ρ_w = density of water; ρ_c = density of unhydrated cement particles). In the former range, the cement paste is considered as a collection of unhydrated cement particles with modulus of elasticity E_u embedded in partially hydrated cement gel with $E_m = 27200r$ (MPa) where r is the relative degree of hydration. The volume fraction of unhydrated cement particles is

$$V = \frac{1 - 0.83r(w/c)(\rho_c/\rho_w)}{1 + (w/c)(\rho_c/\rho_w)} \tag{10}$$

and

$$\Theta = 0.5\left[\kappa_u \sqrt{1-V}(1-n) + \sqrt{\kappa_u^2(1-V)(1-n)^2 + 4n}\right] \tag{11}$$

where κ_u is a shape factor of an unhydrated cement particle. For $w/c > 1.2\rho_w/\rho_c$, the cement paste is regarded as a collection of capillary pores embedded in solid, hydrated cement gel. Now, $n = 0$, $\Theta = \kappa_k(1 - V)$ with κ_k being a shape factor of a capillary pore and the volume fraction of capillary pores

$$V = \frac{w/c - 1.2r\rho_w/\rho_c}{w/c + \rho_w/\rho_c} \tag{12}$$

For mortar ($E = E_r$), $E_m = E_p$, n is the ratio of modulus of elasticity of the fine aggregate particles E_s to E_p and $V = V_s$. Moreover,

$$\Theta = \frac{1}{2}\left[q + \sqrt{q^2 + 4n}\right] \tag{13}$$

Here, $q = \kappa_s(1-V_s)+n\kappa_s(V_f-1)$ and $\kappa_s = 3A_s(1+A_s)/(1+A_s+4A_s^2)$ with A_s being the aspect ratio of the fine aggregate particles.

For plain concrete, $E_m = E_r$, $n = E_c/E_r(1-\beta^{7.5/(5+E_c/E_r)})$ with E_c the modulus of elasticity of the coarse aggregate particles and Θ is given by equation (13) after replacing V_s with V_c, κ_s with κ_c, and A_s with A_c. V_c is the volume fraction of coarse aggregate, κ_c is the shape factor of coarse aggregate particles, A_c is their aspect ratio, and β is the surface area of debonded coarse aggregate relative to its total surface area.

3 Micromechanical relations for fibre-reinforced concrete

The specific fracture energy is

$$G_F = \frac{h}{24}\, L^2\, V_f\, \alpha\, \eta\, K_{Ic,p}\sqrt{\frac{1}{d}\frac{E_f}{E_m}} \tag{14}$$

where $h = \frac{2}{4+f^2}(e^{f\pi/2}+1)$ is the snubbing factor, $K_{Ic,p}$ the fracture toughness of the paste, f the snubbing friction coefficient, α an empirical constant and η the toughening ratio of the matrix.

The direct tensile strength is given by

$$f_t' = \frac{h}{4}\, L\, V_f\, \alpha\, \eta\, K_{Ic,p}\sqrt{\frac{1}{d}\frac{E_f}{E_m}}\,\frac{\delta}{\delta_o} + f_{t,b}'(1-V_f) \tag{15}$$

where the effective deformation of the localization zone δ and the maximum opening of the cracks in the localization zone δ_o at the attainment of f_t' are determined numerically as proposed by Lange-Kornbak & Karihaloo (1997). The direct tensile strength of the composite exclusive of the fibres $f_{t,b}'$ follows from eqn (2).

The uniaxial compressive strength is derived from

$$f_c' = \max \frac{\frac{2}{\sqrt{2}c}\sqrt{b\sin\left(\frac{\pi u}{b}\right)}K_{Ic}(u) + 2\tau_B}{1-\mu} \tag{16}$$

by letting u increase incrementally. c, b and u refer to the configuration of the well-known wing cracks produced in uniaxial compression; u is the half- length of the individual cracks, b the crack spacing and c the half-length of the inclined portion of the individual cracks measured in the direction of the applied compressive stress. μ is the coefficient of friction of the crack surfaces and

$$\tau_B = \frac{h}{4}\, L\, V_f\, \alpha\, \eta\, K_{Ic,p}\sqrt{\frac{1}{d}\frac{E_f}{E_m}}\,\frac{\delta}{\delta_o} \tag{17}$$

The fracture toughness of the fibre composite $K_{Ic}(u)$ is estimated as outlined by Lange-Kornbak & Karihaloo (1997).

Having determined the modulus of elasticity of the matrix phase in a fibre-reinforced composite from expressions (9) – (13), formula (9) can again be used to find E of the fibre composite. Now, let the volume fraction of fibre $V_f = V$ and

$$\Theta = \frac{1}{2}\left\{\kappa + n\kappa' + \sqrt{(\kappa + n\kappa')^2 + 4n(1-\kappa-\kappa')}\right\} \tag{18}$$

in which $\kappa = \kappa_o(c_d - V_f)c_d$, $\kappa' = \min\left(\kappa_o(V_f - c_D)/c_d, 1\right)$, $\kappa_o = 3A(1+A)/(1+A+4A^2)$, $c_d = \kappa_o/(1+\kappa_o)$, $c_D = (2c_d)^{10}/2$, $A = L/d$ and $n = E_f/E_m$, where L is the length and d the diameter of the fibres.

4 Optimum mix compositions

It has been found that mixes attain the same optimum combinations of microstructural parameters when employing either of the following two design criteria, Lange-Kornbak & Karihaloo (1996, 1998): (i) simultaneous maximization of the characteristic length and direct tensile strength for a prescribed compressive strength; (ii) maximization of the characteristic length (i.e. minimization of $-l_{ch}$) alone for a prescribed compressive strength. The most efficient design approach is to formulate a single-criterion optimization problem as follows: For a prescribed f_c',

$$\text{Minimize} \quad -l_{ch}(\mathrm{x}) \tag{19}$$

by choosing the vector of microstructural parameters $\{\mathrm{x}\}$ in such a way as to meet the micromechanical relations for E, G_F, f_t' and f_c', as well as upper and lower bounds on $\{\mathrm{x}\}$. To illustrate this, consider a plain concrete mix with microstructural parameters satisfying the bounds

$$0.2 \le w/c \le 0.45 \tag{20}$$

$$4.0\,\text{mm} \le g \le 32.0\,\text{mm} \tag{21}$$

$$0.005 \le V_c, V_s \le 0.6 \tag{22}$$

and $\nu = 0.2$; $g_{av} = 0.25g$; $f_{t,a}' = 10\,\text{MPa}$; $r = 0.75$; $E_u = 75000\,\text{MPa}$; $\kappa_u = 1.0$: $\kappa_k = 0.7$; $E_s = E_c = 65000\,\text{MPa}$; $A_f = A_c = 1.0$; $\beta = 0.2$; $\xi = 10 \cdot 10^{-6}\,\text{m}$; $\tau = 2.5\,\text{MPa}$; $(\lambda, \gamma) = (0.39, 0.22)$; $g' = 0.01g$; $V_{air} = 0.02$ and $\rho_c = 3150\ \text{kg/m}^3$.

Also consider a fibre-reinforced DSP mix having

$$0.1 \le V_s \le 0.7 \tag{23}$$

$$1.5\,\text{mm} \le g \le 4.0\,\text{mm} \tag{24}$$

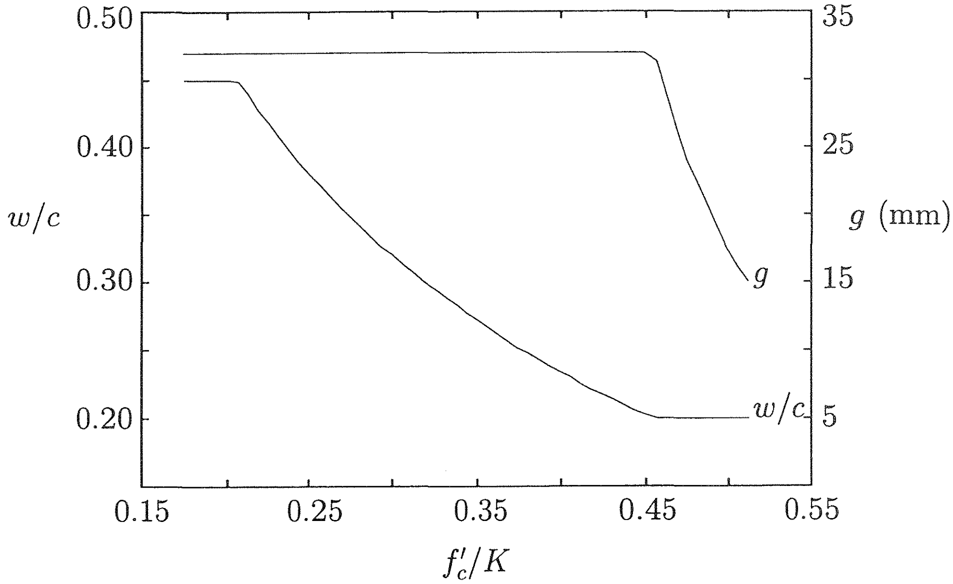

Fig. 1. Optimum water/cement ratio and coarse aggregate size versus relative compressive strength for plain concrete

$$3.0\,\text{mm} \le L \le 20.0\,\text{mm} \tag{25}$$
$$0.1\,\text{mm} \le d \le 0.5\,\text{mm} \tag{26}$$
$$0.01 \le V_f \le 0.16 \tag{27}$$
$$0.4\ \text{MPa}\sqrt{\text{m}} \le K_{Ic,p} \le 1.0\ \text{MPa}\sqrt{\text{m}} \tag{28}$$

and $\alpha = 500\,\text{m}^{-1}$; $g_{av} = 0.375g; \mu = (1 + 0.2g)/3\,(g\,\text{in mm}); e = g_{av}(V_s^{-1/3} - 1); c = \sqrt{2}(0.75g + e/4); b = 0.1346V_s g; W = (3.0g + e)/(0.18 + 3.4V_f); f = 0.9$.

The optimum combination of microstructural parameters is shown in Figs 1 and 2 for plain concrete mixes and in Figs 3 – 5 for fibre-reinforced DSP mixes. For $f'_c/K < 0.212$, the optimal plain concrete mixes have $w/c = 0.45$ and $g = 32$ mm (Fig. 1), while V_c and V_s vary, as shown in Fig 2. For $f'_c/K \ge 0.212$, V_c and V_s attain the upper bound of 0.6, while w/c and g vary, as shown in Fig. 1. For the optimal fibre-reinforced DSP mixes it can be seen that the aggregate properties (Fig. 3) and those of the paste represented by $K_{Ic,p}$ (Fig. 4) essentially remain constant in the entire range of f'_c studied here; $V_s = 0.7, g = 4.0$ mm and $K_{Ic,p} \approx 0.44$ MPa$\sqrt{\text{m}}$. Therefore, the most effective means of controlling the properties of the DSP mix appears to be the variation of the fibre properties V_f and L/d, cf. Figs 4 and 5, respectively. To increase f'_c, the fibre aspect ratio L/d will quickly increase towards its maximum value, while the volume fraction of fibre V_f will increase steadily.

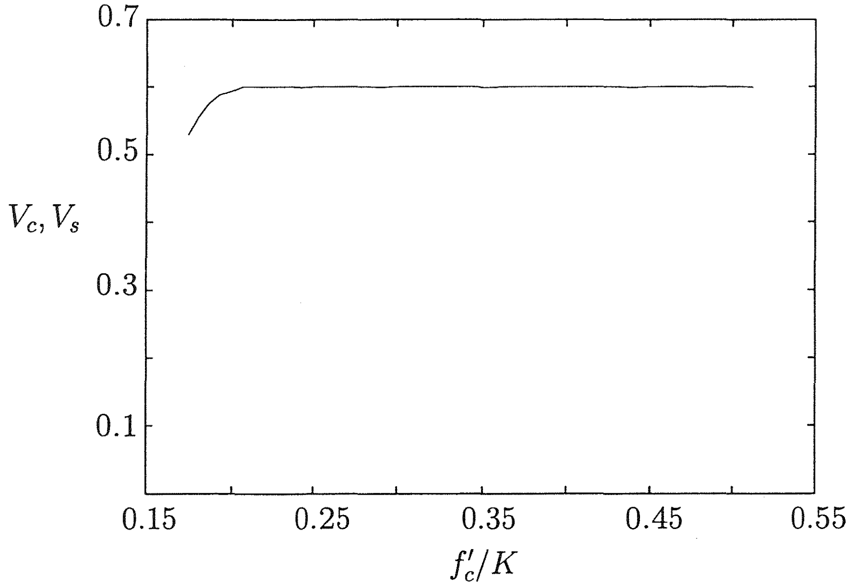

Fig. 2. Optimum volume fractions of coarse and fine aggregate (which are equal $V_c = V_s$) versus relative compressive strength for plain concrete

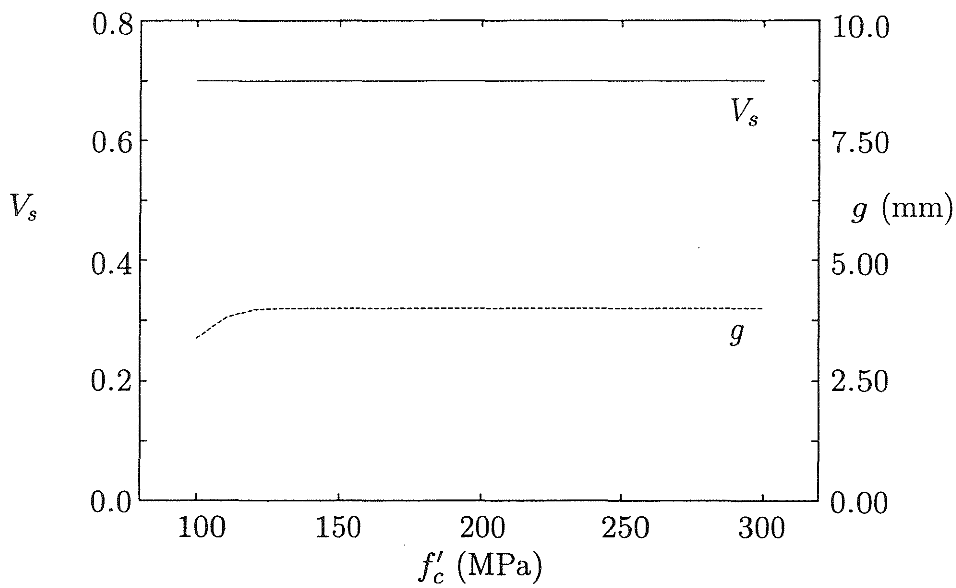

Fig. 3. Optimum volume fraction of fine aggregate and fine aggregate size versus compressive strength for fibre-reinforced DSP mortar

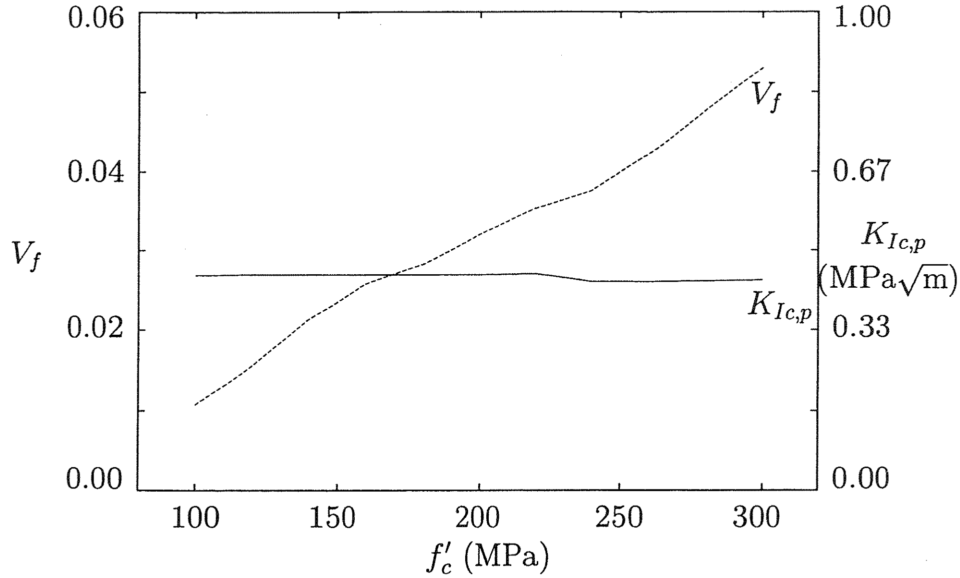

Fig. 4. Optimum volume fraction of fibre and fracture toughness of paste versus compressive strength for fibre-reinforced DSP mortar

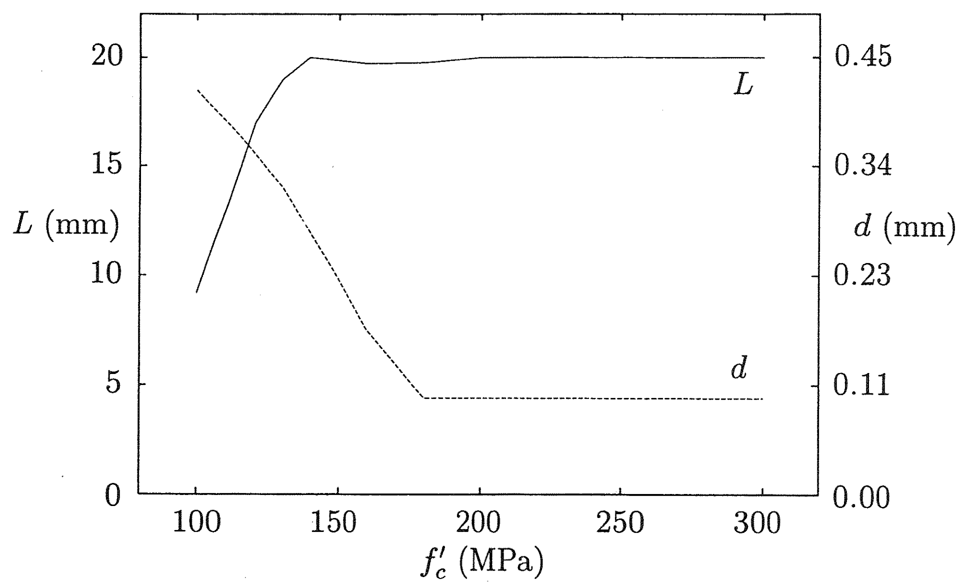

Fig. 5. Optimum length and diameter of fibre versus compressive strength for fibre-reinforced DSP mortar

5 Conclusions

The present study demonstrates that plain and fibre-reinforced concrete mixes can be rigorously designed for overall properties by applying the principles of mathematical optimization. For plain concrete mixes, the maximum characteristic length is achieved for mixes with high volume fractions of coarse and fine aggregates ($V_c = V_s = 0.7$), a high water/cement ratio and a large coarse aggregate size. The most favourable way to attain the required compressive or direct tensile strength is by varying the water/cement ratio; the next most favourable way is by varying the maximum coarse aggregate size.

For fibre-reinforced DSP mixes, the optimum (maximum) characteristic length at any prescribed compressive strength is attained by mixes with a high content of the fine aggregates ($V_s = 0.7$), moderate toughness of the paste ($K_{Ic,p} \approx 0.44$ MPa$\sqrt{\text{m}}$), large size of the fine aggregates ($g = 4$ mm) and low to moderate content of fibres ($V_f \leq 0.055$). The most favourable way to attain the required compressive or direct tensile strength of a fibre-reinforced DSP composite is by varying the properties of the fibres. Thus, to gain additional strength, the fibre aspect ratio and the volume fraction of fibre must be increased.

6 References

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