# Predicting Joint Sealant Performance of Elastomers by Computer Simulation. III. Simulation of Single- and Multi-Step Extension of a Stress-Relaxing Material

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#### Synopsis

Computer simulation of the extension of a joint seal that had fully relaxed in a compressed configuration indicated that exceptionally high stresses were engendered if the extension occurred in a single step, as provided in certain "performance tests." When the same amount of extension was simulated by a stepwise procedure, with the assumption of full relaxation after each step, not only were the stresses smaller, but the stress concentration factors in the extreme corners of the joint seal were much reduced, so that the likelihood of failure under such conditions would appear to be remote. This stepwise extension pattern is considered to be more representative of real joint behavior than the "accelerated performance test."

## INTRODUCTION

Sealants in "dynamic" joints (in buildings and other structures) are compelled to undergo a wide variety of movements at various rates. In attempting to assess the probable performance of a given material in a particular use, considerable insight can be obtained by computer simulation of the response of the material in the appropriate configuration.<sup>1-3</sup> An available computer program has been slightly modified and can be used in the following conditions:

1. The sealed joint is long, straight, and of uniform cross section. (Considerable latitude is permitted as to shape of cross section.)

2. All joint movement and applied forces are perpendicular to the joint length, but a *uniform* stretching or compression (such as would result from thermal expansion of the structure) can be imposed along the joint length.

3. The sealant material can be prepared in some form suitable for simple laboratory tests, e.g., sheets or rings.

4. Joint movements may be analyzed into motions that can be studied in the laboratory, e.g., constant-strain-rate deformation, stress relaxation at constant deformation, or creep under constant load. These motions may be applied in sequence, provided the effects can be superimposed. This latter provision is checked in the laboratory also.

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Fig. 1. Predicted half-section of  $\frac{1}{2}$ -in. square model sealed butt-joint compressed 25%, confined between walls. Sealant A compressed 40%/min at 70°F.

5. Body forces (e.g., weight) and a fairly complex system of in-plane forces (e.g., pressures and shears) may be imposed.

6. The presence of certain kinds of reinforcing elements, holes, or other heterogeneities may be provided for.

In response to thermal expansion-contraction of the adjacent structural elements, joint seals undergo cyclic compression-extension. Materials that undergo no stress relaxation (e.g., the silicone-based sealant B of our first paper<sup>2</sup> obviously can be simulated without consideration of past history, if the assumption is made that their properties do not change on aging. Materials that relax stress require a more sophisticated approach; we are developing this approach by stages.

The next simplest simulation is to assume a material that relaxes stress completely (after a suitable time-temperature sequence) but which retains the short-time elastomer-like properties that it had before stress relaxation. Many laboratory studies have shown that polysulfide-based sealants behave approximately this way.<sup>4</sup> The joint seal configuration chosen for calculation was that specified in the Interim Federal Specifications<sup>5,6</sup> for cyclic testing of sealants:  $\frac{1}{2}$  in.  $\times \frac{1}{2}$  in. The computation assumes an infinite length, and we have found that a 6-in. length is satisfactory;<sup>3</sup> but the specifications call for only a 2-in. length, so our computation is somewhat more demanding in this respect.

## **COMPUTER SIMULATION: ONE-STEP EXTENSION**

The first step in the simulation was to calculate the shape of the joint seal cross section after 25% compression at room temperature. Since such a computation had already been obtained (at 0.2 ipm) for a simplified polysulfide sealant (sealant A of our previous paper), this material was chosen

The shape of the compressed joint seal (assumed for further computations. to be a recessed seal) is shown in Figure 1. Note that the sealant has been forced into contact with the substrate above the original filling line. It seems unlikely that the already cured sealant would adhere firmly to the substrate in this region, so no adhesion was assumed for further calcula-The other needed assumptions have already been stated: after tions. enough time has passed, the compression stresses have relaxed completely and the material still has the same fundamental properties that it had when (The latter assumption is used only to obviate the need to age first cured. ring samples of the sealant and determine constant-strain-rate properties of the aged material.) The next step in the simulation thus used the shape of Figure 1 as a starting configuration with the material parameters of sealant А.

For the rapid-extension case, this shape was stretched at 0.2 ipm for 1.25 min., producing the deformation required in the Interim Federal Specifications, but at 96 times the rate. The resultant stress distribution is shown in Figure 2.

The most striking features of the reextended joint are the wrinkle on the surface of the stretched joint seal and the very high stress concentration and peeling forces in the corner. The wrinkle is of the same dimensions as the mesh size of the finite-element grid in the corner, so it is rather poorly resolved; but its existence corresponds to observations of cyclically flexed joints, so it may well be a real phenomenon.

The calculated stress in the extreme corner of the joint seal is about three times as high as would be calculated if the original joint had simply been stretched 67%, and it is probably six to eight times the calculated stress if the original joint were simply stretched 25%. The latter situation would arise if the material was fully elastic, so there would be no stress relaxation in the compressed joint seal, and the subsequent extension could be regarded as starting from zero when the joint width again reached 0.500 in.

#### MULTI-STEP EXTENSION

This computation shows that this compression-extension cycle is far more rigorous when applied to a chemorheologically stress-relaxing sealant (particularly one of abnormally high modulus, such as sealant A) than when applied to a nonrelaxing material. An obvious objection to this test is that real joint movements are not nearly so rapid and are more likely to occur in small steps with periods of stress relaxation in between. To simulate the latter situation, the compressed shape (Fig. 1) was again used as a starting point, and the same cross-head speed (0.2 ipm) was provided, but the successive steps were only 0.025 in. each (0.125 min). In this simulation, it was assumed that *complete* stress relaxation occurred after each 5% step, so that the unstressed shape at (net) 20% compression would be the starting point for the second step, that at (net) 15% compression would be the starting point for the third step, etc.







Fig. 3. Successive stepwise extensions of a compressed joint seal. Sealant A at 70°F, 0.2 ipm. Fully stress-relaxed at each step.

The calculated successive shapes of a quarter-section are shown in Figure 3. One wall of the joint has been held fixed while the other wall (and hence the centerline) has been moved away. The uppermost shape, at 25% compression, shows the nonadherent region of material pressed against the wall above the original filling level. As this is pulled away from the wall, a distinct wrinkling of the free surface appears and then is partially pulled out. While the exact shape of the wrinkling is undoubtedly dependent on the "grain size" of the finite-element grid used in the computation, its persistence and extent appear to indicate a definite computational prediction of such an effect.

The computed stepwise stresses are summarized in Table I; the next-tolast line gives the result of the one-step extension previously described. Several very striking results appear. Since each step is only one tenth the size of the earlier computation, it is scarcely surprising that the stresses are much smaller. Most noteworthy are the lower stress concentration factors for the stepwise procedure. That is, the ratio of the principal tensile stress in the corner to the nominal tensile stress in the joint is far less and decreases with each subsequent step. Naturally, the nominal stress in the joint seal at 25% extension is greatly reduced by the intervening relaxations, but the considerable drop in stress for each succeeding step is a bit surprising. Explanation includes the smaller depth at the centerline for the later steps and the smaller fraction of the relaxed joint width represented by these latter steps. Note that even a direct summation of the nominal stresses for all ten steps gives less than the nominal stress computed for a single large

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 Job no.	"Extended," <sup>b</sup> %	Max. "bulge- up," <sup>°</sup> in.	Centerline tensile stress, <sup>d</sup> psi nominal	Max. principal tensile stress,• psi	Stress <sup>f</sup> concentra- tion factor
Start	-25	0.1025		<u> </u>	
102969-1	-20	0.0803	23.4	82.1	3.51
103069-1	-15	0.0591	21.2	71.0	3.35
103169-1	10	0.0392	19.4	65.4	3.37
110469-1	-5	0.0208	17.7	55,9	3.16
111269-1s	0	0.0040	16.0	51.8	3.24
111469-1	+5	-0.0113	14.4	41.1	2.86
111769-1	+10	-0.0252	13.0	32.2	2.48
111869-1	+15	-0.0377	11.8	$27.6^{ m h}$	2.34
112069-1	+20	-0.0491	10.6	24.7 <sup>h</sup>	2.33
112669-1	+25	-0.0594	9.65	22.1 <sup>h</sup>	2.29
010469-1 <sup>3</sup>	$+25^{i}$	-0.0535	176.3	1375.0	7.80
111970 <sup>j</sup>	$+25^{i}$	-0.0535	119.8	932.5	7.80

TABLE I						
Predicted Behavior of a Bulged Joint in Stepwise	Extension					

• Sealant A, 70°F, fully stress-relaxed. Cross-head speed, 0.2 ipm, except where noted. All predictions at next-to-last iteration.

<sup>b</sup> Referred to original width; compression is negative.

• Displacement from original filled level at centerline; downward displacement is negative.

 $^{\bar{d}}$  Referred to 0.5" depth adhering to wall; "centerline" refers to location of summed stress elements.

• In corner of joint seal unless otherwise noted.

<sup>f</sup> Max. principal tensile stress/nominal tensile stress in joint seal.

<sup>s</sup> Grid layout redefined before this job.

<sup>h</sup> In element in outermost layer, one removed from corner of joint seal.

<sup>i</sup> One-step extension at 0.2 ipm from -25%.

<sup>i</sup> One-step extension at 0.125 iph from -25%.

step at the same rate. This crude application of a superposition principle is clearly not justified in this "large deformation" situation.

The stress concentrations resulting from the joint seal shape are even more substantially reduced by allowing full stress relaxation between steps. The resulting stress concentration factors become relatively mild. It is also noteworthy that the point of maximum stress eventually moves away from the extreme corner of the joint into the beginning of the wrinkled region. This effect is, perhaps, a function of the "grain size" of the computation, but there appears to be a clear effect of spreading out and reducing the intensity of the most highly stressed region which may be important in predicting the locus of failure initiation. The principal stress "isodynics" for the last step are plotted in Figure 4 and are shown with greater detail in Figure 5. These stress distribution patterns may be compared directly with Figure 2; the same cross-head speed was simulated in both cases.

Note, however, that the Interim Federal Specifications (I.F.S.) test provides that the standard test joint be compressed 25%, held at  $158^{\circ}$ F for a week, and then cycled between 25% compression and 25% extension, at a



Fig. 4. Predicted shape and stress distribution at 25% extension. Sealant A at  $70^{\circ}$ F,  $\frac{1}{2}$ -in. square cross section, confined. Compressed 25% at 0.2 ipm and fully stress-relaxed, then reextended in 5% steps at 0.2 ipm to 25% greater than original width. Full stress relaxation after each step. Isodynics in psi.



Fig. 5. Corner detail of Fig. 4.

speed of 0.125 in./hr, which is about 1% of the rate used in both the simulated one-step extension and the ten-step simulation. It might well appear that the slowed cycling speed would allow relaxation and thus compensate for the large single jump applied without periods of relaxation. To see how much effect the I.F.S. cycling speed would have, the one-step extension was recomputed. To get the effective speed down, it was necessary to provide a 2-hr isochrone from the data measured at rates from 0.2 ipm to 50 ipm on ring samples of the sealant. This was done by assuming that the same linear relationship between log time and log stress at a given extension that was found for 0.01 to 20 min (see Fig. 2 of Catsiff et al.<sup>2</sup>) would hold to 2 hr.

The results of this "slow one-step" computation are given in the last line of Table I. Although the reduced speed does permit some relaxation of the stresses involved, the stress concentration factor remains high, and the peak stress to be expected is still more than ten times as high as those encountered if the reextension were to occur in small steps with sufficient stress relaxation between steps, even though the speed of the separate short steps was nearly 100 times as fast (0.2 ipm). Thus, the attempt to "accelerate" the I.F.S. test by continuous cycling favors nonrelaxing sealants, whereas stressrelaxing sealants do well in situations that resemble actual sealed joint

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behavior, i.e., the behavior to be expected in a dynamic joint undergoing annual climatic or daily temperature cycling.

It seems reasonable to conclude that a compression-extension cycle which provides small increments of deformation, with periods of stress relaxation between increments, is a very mild test for a chemorheologically stressrelaxing material, even if the total deformation is considerably greater than  $\pm 25\%$ . For a nonrelaxing material, only the overall amount of deformation is significant; if this is large, no matter how slow the rate of attainment, a severe requirement is imposed.

#### References

1. E. H. Catsiff, R. F. Hoffman, and R. T. Kowalewski, Adhesives Age, 13(3), 21 (March 1970).

2. E. H. Catsiff, R. F. Hoffman, and R. T. Kowalewski, J. Appl. Polym. Sci., 14, 1143 (1970).

3. E. H. Catsiff, R. F. Hoffman, and R. T. Kowalewski, J. Appl. Polym. Sci., 14, 1159 (1970).

4. M. D. Stern and A. V. Tobolsky, J. Chem. Phys., 14, 93 (1946).

5. Interim Federal Specification TT-S-00230b (COM-NBS), Section 4,3,9, Sept. 25, 1968.

6. Interim Federal Specification TT-S-00227D (COM-NBS), Section 4,3,9, Oct. 23, 1968.

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