

Mechanism of Antifoaming Action of Simethicone

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The mechanism of the foam-inhibiting action of simethicone, mainly used against flatulence, has been studied. Its effect on foaming systems containing synthetic gastric juice and a surface-active substance (anionic surfactant, cationic surfactant, soap solution) was quantitated by measuring the surface tension, foam stability and initial foam density. The effect of simethicone on each of the examined systems was the result of the combination of two actions: the drainage of liquid from foam films and the rupture of relatively thick liquid films. The mechanism of these actions may be described as the liquid drainage followed by bridging of the liquid film by polydimethylsiloxane droplets, helped by hydrophobic silica particles also present in the antifoaming agent, leading to the rupture of the film surface and air escape.

INTRODUCTION

Poisoning caused by foaming detergents is rare. However, when it does happen urgent action is needed. Not only does the ingestion of a detergent (mainly cationic) increase the absorption of toxic substances from the gastrointestinal tract but it also brings about irritation of the gastric mucous membrane and through vomiting it can even intensify the foaming of the detergent. This may lead to detergent aspiration, aspiration pneumonia, pulmonary oedema and finally respiratory blocking and suffocation. The most imperilled individuals in such cases are children.¹⁻³ Immediate and appropriate use of an antidote may save the patient from death.

Simethicone is an agent that is widely used and has been known for a considerable time. It is a chemically inert mixture of polydimethylsiloxane ((CH₃)₂[Si(CH₃)₂O]_n) and silica gel, it is physiologically inactive and is not toxic if used orally. Investigations have shown that simethicone is hydrophobic and stable at elevated temperature. Based on its property to decrease the surface tension of a liquid, some authors⁴ consider that simethicone can prevent bubble formation and gas retention in the foam and can help to eliminate flatulence. Like some other silicone agents, simethicone is mainly used as an antifatulence agent.⁵⁻⁷ It is also recommended by the Swiss Toxicology Information Centre (Schweizerisches Toxikologisches Informationszentrum)⁸ as an antifoaming agent that is efficient after the ingestion of detergents. However, simethicone has been classified by the International Programme on Chemical Safety (IPCS) and the Commission of the European Community (CEC) as a widely used antidote requiring further research.⁹

The aim of this study is to investigate the effect of simethicone on some foaming liquids widely used in

the household and to explore the mechanism of its foam-inhibiting action.

EXPERIMENTAL

Different foaming systems were prepared. Each system consisted of a synthetic gastric juice and a surface-active substance (added in the form of a liquid detergent for washing up, a surface cleaning agent or a 1 vol.% aqueous soap solution) with or without the addition of the antifoaming agent simethicone.

The synthetic gastric juice was prepared by dissolving 2 g of sodium chloride and 3.2 g of pepsin in 1 l of bidistilled water. The solution was adjusted to pH 1.2 with hydrochloric acid.¹⁰ The chemicals (namely sodium chloride and hydrochloric acid) were of analytical grade and water was a bidistillate. The pepsin employed was a pharmaceutical grade product prepared as in Ref. 10.

Simethicone, baby soap, washing-up liquid and surface cleaning agent were standard products, all commercially available. The baby soap was a sodium salt of animal and vegetable fatty acids, the washing-up liquid contained an anionic synthetic surfactant, sodium dodecyl benzene sulphonate, and the surface active ingredient of the surface cleaning agent was a quarternary cationic surfactant, hexadecyltrimethylammonium bromide.

Surface tension, initial foam density and foam stability measurements were made on systems containing 1 vol.% and 5 vol.% surface-active agent. If not otherwise stated, simethicone was added into the systems in a concentration of 1.5 vol.%.

The surface tension of the solutions was measured at 37 ± 0.5 °C by means of a Lecomte du Noüy tensiometer (Krüss, Hamburg). Several measurements were done at intervals up to 30 min.

The initial foam density and the foam stability were determined in the manner described by Ross and Young,¹¹ which is suitable for aqueous foams with a

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rather short lifetime. Freshly prepared foam, obtained after mechanical stirring of 200 cm³ of sample for 5 min at maximum speed, was filled top-flat in a previously weighed 10-cm³ sample bottle. The sample bottle together with the contents was then weighed again to determine the foam density. The deviation of the measurements was within 2%.

To measure the foam stability the freshly whipped foam, prepared as described, was transferred within a few seconds into a 250-cm³ graduated cylinder up to the highest gradation. The observation of liquid drainage and air escape from the foam was followed until no further change could be measured. All measurements were performed at a room temperature of 25 °C with an average deviation of < 1 °C.

The foam stability was characterized by the average lifetime of air (L_a) and liquid (L_l) in the foam, defined by the equations¹¹

$$L_a = 1/(v_a)_i \int_0^{(v_a)_i} t \, dv_a \quad (1)$$

and

$$L_l = 1/(v_l)_i \int_0^{(v_l)_i} t \, dv_l \quad (2)$$

and the average lifetime of foam (L_f)

$$L_f = 1/(v_f)_i \int_0^{(v_f)_i} t \, dv_f \quad (3)$$

where v_a , v_l and v_f are the volumes of air, liquid and foam at time t , respectively, the total volume of the foam $v_f = v_a + v_l$ and the initial volumes are marked with i .

As the relative foam density is

$$d_f = v_l/v_f \quad (4)$$

the average lifetime of the foam can be calculated from the equation

$$L_f = L_a + d(L_l - L_a) \quad (5)$$

derived from Eqns (3) and (4), where d refers to the initial relative foam density

$$d = (v_l)_i/(v_f)_i \quad (6)$$

To determine L_l the observations were made at the foam/liquid interface, and to determine L_a at the foam/air interface.

RESULTS AND DISCUSSION

The selection of foaming systems was based on the requirement to study the nature of the effect of the chosen antifoaming agent on currently used products that provide stable foam. The foam stability measurements in the presence of simethicone were performed at a concentration below that customarily prescribed

Table 1. The effects of 0.01 vol.% simethicone on initial foam density (d_i) and initial volume of liquid in the foam ($(v_l)_i$) in the tested systems

System	Surfactant concentration (%)	d_i (g cm ⁻³)	$(v_l)_i$ (cm ³)
Anionic surfactant	1	0.080	41
	5	0.354	70
Anionic surfactant with simethicone	1	0.517	127
	5	0.808	155
Cationic surfactant	1	0.133	80
	5	0.248	91
Cationic surfactant with simethicone	1	0.483	100
	5	0.495	113
Soap solution	1	0.092	56
Soap solution with simethicone	1	0.446	103

(~ 1.5 vol.%), so that sufficient foam was produced. Therefore, the concentration of the agent was reduced to 0.01 vol.%, which permitted a relatively stable foam formation. As observed, the initial foam density (d_i) and the initial volume of liquid in the foam of all the examined systems increased with the addition of the antifoaming agent (Table 1). In systems containing the antifoaming agent in a concentration far from that of complete inhibition, as was the case here, this is a common phenomenon.¹¹

The surface tension of the systems was also affected by the addition of simethicone (Table 2), although the surface tension was already low because of the presence of surface-active substances. Polydimethylsiloxane, one of the constituents of simethicone, is known to have a very low surface tension not exceeding 21 mN m⁻¹ at room temperature.¹²

Typical curves showing the rate of separation of liquid and air from the foam, with and without the presence of the antifoaming agent simethicone, are demonstrated in Fig. 1. In the initial period air separation was not noticeable. This period is also characterized by a liquid outflow, which is more rapid at the beginning of the drainage. After further shrinkage the film ruptures and air escapes from the foam, as shown

Table 2. Surface tension of synthetic gastric juice at 37 °C with the standard deviation for the examined foaming systems

Additions	σ (mN m ⁻¹)
None	51.27 ± 1.16
Simethicone	28.58 ± 0.30
1% Anionic surfactant + simethicone	29.20 ± 0.00
5% Anionic surfactant + simethicone	25.07 ± 0.06
1% Cationic surfactant + simethicone	29.05 ± 0.06
5% Cationic surfactant + simethicone	24.45 ± 0.17
1% Soap solution + simethicone	38.73 ± 0.26
5% Soap solution + simethicone	29.37 ± 0.15
1% Soap solution + simethicone	36.73 ± 0.10
5% Soap solution + simethicone	28.98 ± 0.10
1% Soap solution + simethicone	38.85 ± 0.13
5% Soap solution + simethicone	25.23 ± 0.19

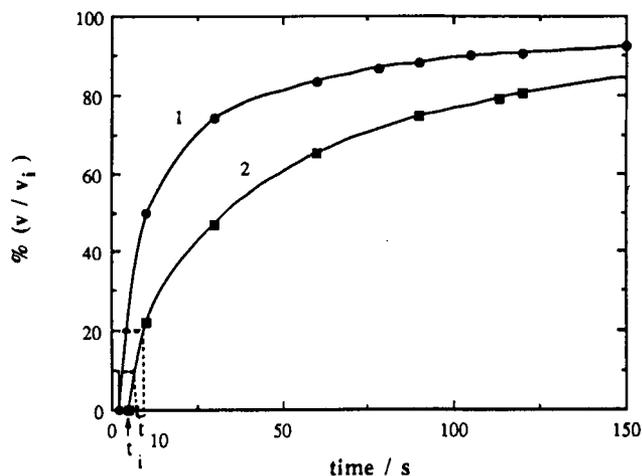


Figure 1. Rate of air (a) and liquid (b) separation from foams containing 1 vol.% cationic surfactant in the presence (1) and absence (2) of simethicone.

by a rapid change in the volume of air in foam vs time curve. In the presence of simethicone, the initial period of foam stability is much shorter and the process of liquid film rupture starts at a larger liquid content in the foam and proceeds at an increased rate.

The influence of simethicone is even more marked on changes of foam density with time. These values can be evaluated, as proposed by Ross and Young,¹¹ from the volumes of air, (v_a) and liquid (v_l) in the foam measured at the same time, and from the liquid density (d_l)

$$d_t = v_l \cdot d_l / (v_l + v_a) \quad (7)$$

Figure 2 compares the data for a cationic (A) and an anionic (B) surfactant-containing system. The minimum foam density in the presence of simethicone (curves 2) lies at higher values than in pure foaming systems (curves 1). This difference is larger in the cationic (Fig. 2A) than in the anionic surfactant system (Fig. 2B) because the cationic surfactant foam has a higher air/water surface tension (Table 2) and drains faster than the anionic surfactant foam. The very low

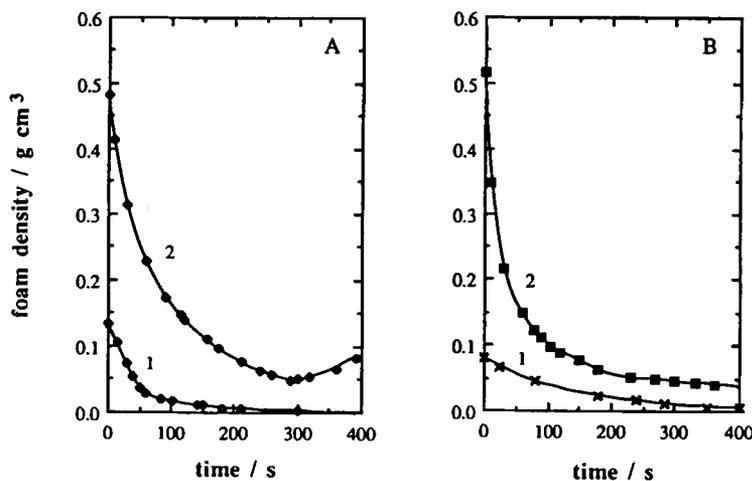


Figure 2. Changes in foam density with time for 1 vol.% cationic (A) and 1 vol.% anionic (B) surfactant-containing system without (curve 1) and with (curve 2) simethicone.

Table 3. Effect of simethicone on foam stability of the examined foaming systems

Foaming system	Surfactant concentration (%)	L_1 (s)	L_a (s)	L_f (s)
Anionic surfactant	1	132	2173	1838
	5	84	2548	1858
Anionic surfactant with simethicone	1	71	621	342
	5	54	1103	453
Cationic surfactant	1	43	1872	1287
	5	71	2244	1453
Cationic surfactant with simethicone	1	80	403	282
	5	91	470	299
Soap solution	1	98	2068	1627
Soap solution with simethicone	1	85	502	330

concentration of simethicone used in these experiments may be the reason for the effect not being even more pronounced. Yet, the values for the foam density obtained in the presence of the antifoaming agent suggest that the drainage of liquid from the foam is still the predominant action in the destabilization of the liquid films in both systems, although it is less pronounced in the cationic surfactant-containing systems. When the minimum density value is reached the drainage is practically nil and the escape of air from the foam, as a consequence of the film rupture, becomes dominant (Fig. 1). Such a reversed relation between the mass and the volume of the foam may even cause an increase in foam density (Fig. 2A, curve 2).

A comparison of foam stabilities in the form of numerical indices L_1 , L_a and L_f for the examined systems is given in Table 3. The values of L_a and L_1 give the information about the nature of the foam, measuring directly the film stability and the rate of film drainage, respectively, and giving thus the information about the role of film rupture and liquid drainage in foam stability. The index L_f incorporates both these values. In the cases presented here the

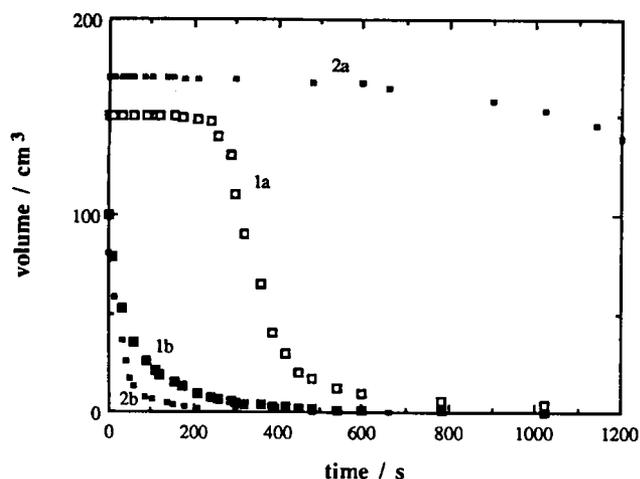


Figure 3. Separation of liquid from the foam (vol.%) as a function of time for 1 vol.% anionic (1) and 1 vol.% cationic (2) surfactant system in the presence of simethicone.

values of L_a are all greater than those of L_1 , which suggests that the drainage of liquid from the foam in all systems is a more pronounced factor than the film rupture and air escape, especially in thin films before air is trapped in the foam for a relatively long period of time and the liquid separates from the foam at a faster rate than does the air. The values of L_a obtained in the presence of the antifoaming agent are lower than those obtained in its absence. This indicates that the antifoaming agent influences the drainage by causing liquid film rupture while still relatively thick. On the other hand, the presence of simethicone reduces the values of L_1 in anionic surfactant and soap solution systems but increases these values in cationic surfactant systems. This phenomenon could be explained by the assumption that simethicone affects the drainage of the cationic more than the anionic surfactant system, so that a larger volume of liquid present in the anionic surfactant foams separates at nearly the same initial rate or even faster than in cationic surfactant foams.

Koczó and Rácz¹³ proposed a model by which the initial rate of drainage could be expressed as a time that elapsed between the time of the first liquid drop appearance (t_i) and the time needed for 10 vol.% of the foam liquid to drain, measured from the appearance of the first 10 vol.% (t_{10}). Figure 3 compares the effect of simethicone on the initial rate of drainage in a cationic and an anionic surfactant-containing system. The values of t_{10} and t_i for these systems are given in Table 4. The data clearly show that simethicone indeed did not influence the initial outflow rate of liquid from the foam in cationic surfactant systems. What is more, in 1 vol.% cationic detergent systems this process was even retarded. The values of t_i in the systems with the antifoaming agent present were all smaller than in comparable pure foaming systems. This would refer to the rupture of liquid film rather than the increased drainage of liquid from the foam. If so, the value of L_a in these systems should be smaller than the value of L_1 . The tendency of L_a to decrease and L_1 to increase with the addition of simethicone to the cationic surfactant systems supports the assumption that a higher concentration of this agent than that used in these experiments would probably cause the value of

Table 4. Time lag for liquid outflow (t_i) and the rate of liquid drainage (t_{10}) for anionic and cationic surfactant systems

Foaming system	Concentration (%)	t_i (s)	t_{10} (s)
Anionic surfactant	1	13	8
	5	7	4
Anionic surfactant with simethicone	1	2	1
	5	2	2
Cationic surfactant	1	6	3
	5	4	5
Cationic surfactant with simethicone	1	5	4
	5	2	5

L_1 to become even higher than L_a . Indeed, the concentration of 1.5 vol.% simethicone destabilized the existing foam in practically no time. Such behaviour is characteristic for the antifoaming agents to be able to spread on the film surface and destroy the thick films before they drain out.

Our results are in support of such a behaviour of simethicone. The foam stability index (L_f), which comprises both L_1 and L_a values, shows that simethicone has a rather strong antifoaming effect on all the examined foaming systems (Table 3). The addition of the antifoaming agent changed the proportions between these two values in favour of L_1 , because the value of L_a decreased by a factor 3–4 while, at the same time, the value of L_1 did not exceed a factor of 2.

It has already been reported^{14,15} that polydimethylsiloxane alone or in association with hydrophilic silica does not exhibit any antifoaming activity and, even more, at certain surface concentrations it stabilizes liquid films.^{15,16} However, when prepared by an admixture of colloidal hydrophobic silica it acts as a very effective antifoaming agent.¹⁴ This suggests that polydimethylsiloxane and hydrophobic silica act complementary to each other in foam-inhibiting action. The surface properties of polydimethylsiloxane, such as low surface tension, surface viscosity and hydrophobicity, enable this substance to spread easily over a variety of substrates. Thus, droplets of polydimethylsiloxane easily immerse in the foam liquid film and come in contact with both film surfaces by thinning of the liquid film. In that case, as proposed by some recent studies,^{17,18} a bridging of the film by the droplet occurs and the droplet–film contact points then become the places of film rupture. A number of studies^{14,17–21} have focused on explaining the role of the solid in the antifoaming effectiveness of the insoluble liquid, trying to get satisfactory answers with regard to the mechanisms of both their single and mutual action. Because, in our case, the silica particles were dispersed in polydimethylsiloxane, the mechanism of their mutual action, according to some recent studies,^{17,18,20} would most probably be in promotion of the bridging abilities of polydimethylsiloxane by shortening the time required for the film to thin and thus resulting in earlier film rupture.

Naturally, the effect of an antifoaming agent depends not only on its own concentration in the system but also on the physicochemical properties and the

concentration of the surfactant used. As the three examined surfactants have different properties, the intensity of the effect of simethicone varied in each of the comparable systems and most likely depended on the ability of silica particles to enter the surfactant solution.¹⁸ Nevertheless, although the concentration of simethicone used in these experiments was rather low, the mechanism of the antifoaming action could be recognized as a destabilization of the liquid film in an action described above.

CONCLUSION

The antifoaming properties of simethicone, an anti-flatulence agent, have been investigated on three different foaming systems containing anionic surfactant, cationic surfactant and soap solution. The results obtained from the initial foam density, foam stability

and surface tension measurements provided evidence that the bridging of the surfactant liquid films by polydimethylsiloxane, helped and accelerated by the presence of hydrophobic silica particles, thus provoking film rupture while the film was still relatively thick, was the probable mechanism of foam inhibition in all foaming systems. The effect was better pronounced in the cationic than in the anionic and soap solution systems.

These findings are our contribution to the study concerning the efficacy of simethicone as an antidote and antifoaming agent in cases of detergent ingestion and poisoning.

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REFERENCES

1. S. Moeschlin, Alkalimetalle und Erdalkalimetalle. In *Klinik und Therapie der Vergiftungen*, ed. by S. Moeschlin, pp. 207–214. Georg Thieme, Stuttgart (1986).
2. R. Ludwig and K. Lohs, *Akute Vergiftungen*, pp. 418–420. VEB Gustav Fischer, Jena (1988).
3. M. J. Ellenhorn and D. G. Barceloux, *Medical Toxicology*, pp. 897–936. Elsevier, New York (1988).
4. K. Kimura, J. F. Treon and F. R. Benson, Therapeutic use of methylpolysiloxane. *Curr. Ther. Res.* **6**, 202–216 (1964).
5. J.E. Berstein and R. S. Schwartz, An evaluation of the effectiveness of simethicone in acute upper gastrointestinal distress. *Curr. Ther. Res.* **16**, 617–620 (1974).
6. I. A. Bouchier, Flatulence. *Practitioner* **224**, 373–377 (1980).
7. N. K. Jain, V. P. Patel and C. S. Pitchumoni, Activated charcoal, simethicone, and intestinal gas. A double-blind study. *Ann. Intern. Med.* **105**, 61–62 (1986).
8. J. Velvart and A. Nisoli, Antidot-Therapie bei Vergiftungen. *Ther. Umschau* **43**, 250–258 (1986).
9. J. A. Haines and M. Mercier, Mechanism of action and clinical efficacy of antidotes. In *Proc. 5th International Congress of Toxicology*, ed. by G. N. Volans, J. Sims, F. M. Sullivan and P. Turner, pp. 487–505. Taylor & Francis, London (1990).
10. Komisija za farmakopeju. In *Ph Jug.*, 4th Edn, ed. by Zavod za ispitivanje i kontrolu ljekova R. Hrvatske, pp. 199–228. Zagreb (1984).
11. S. Ross and G. J. Young, Action of antifoaming agents at optimum concentrations. *Ind. Eng. Chem.* **43**, 2520–2525 (1951).
12. M. J. Owen, Interfacial activity of polydimethylsiloxane. In *Surfactants in Solution*, ed. by K. L. Mittal and P. Bothorel, pp. 1557–1569. Plenum Press, New York (1986).
13. K. Koczó and G. Rácz, Foaming properties of surfactant solutions. *Colloids Surfaces* **56**, 59–82 (1991).
14. R. D. Kulkarni and E. D. Goddard, Droplet/foam bubble interactions as applied to antifoaming. *Croat. Chem. Acta* **50**, 163–179 (1977).
15. S. Ross and G. Nishioka, Experimental research on silicone antifoams. In *Emulsions, Lattices and Dispersions*, ed. by Becker and Yudenfreud, pp. 237–251. Marcel Dekker, New York (1978).
16. A. A. Trapeznikov and L. V. Chasovnikova, Stabilization of bilateral films by monolayers and thin films of polydimethylsiloxanes. *Colloid J. USSR* **35**, 990–992 (1973).
17. P. R. Garrett, Preliminary considerations concerning the stability of a liquid heterogeneity in a plane-parallel liquid film. *J. Colloid Interface Sci.* **76**, 587–590 (1980).
18. G. C. Frye and J. C. Berg, Mechanisms for the synergistic antifoam action by hydrophobic solid particles in insoluble liquids. *J. Colloid Interface Sci.* **130**, 54–59 (1989).
19. P. R. Garrett, The effect of polytetrafluoroethylene particles on the foamability of aqueous surfactant solutions. *J. Colloid Interface Sci.* **69**, 107–121 (1979).
20. M. P. Aronson, Influence of hydrophobic particles on the foaming of aqueous surfactant solutions. *Langmuir* **2**, 653–659 (1986).
21. G. C. Frye and J. C. Berg, Antifoaming action by solid particles. *J. Colloid Interface Sci.* **127**, 222–238 (1989).