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Application of epidemic models to phase transitions

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Application of epidemic models to phase transitions

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The Susceptible-Infected-Recovered (SIR) and Susceptible-Exposed-Infected-Recovered (SEIR) models describe the spread of epidemics in a society. In the typical case, the ratio of the susceptible individuals fall from a value S_0 close to 1 to a final value S_f, while the ratio of recovered individuals rise from 0 to $R_f = 1 - S_f$. The sharp passage from the level zero to the level R_f allows also the modeling of phase transitions by the number of ''recovered'' individuals $R(t)$ of the SIR or SEIR model. In this article, we model the sol–gel transition for polyacrylamide–sodium alginate (SA) composite with different concentrations of SA as SIR and SEIR dynamical systems by solving the corresponding differential equations numerically and we show that the phase transitions of ''classical'' and ''percolation'' types are represented, respectively, by the SEIR and SIR models.

Keywords: epidemic models; dynamical systems; SIR model; SEIR model; percolation model; sol–gel transition

1. Introduction

The sol–gel transition is a special type of polymerization in which the sol state consists of monomers usually in a solution and the gel state is reached when these monomers are linked *via* physical and/or covalent bonds.

There are two theories that describe this mechanism; the classical or mean-field theory given by Flory and Stockmayer [1–5] and the lattice percolation model [6,7]. These theories differ in the form of the underlying lattice. The Flory–Stockmayer or ''mean-field'' theory is based on a tree-type lattice, i.e., a lattice without closed loops where each node is connected to at most three other nodes and starting from a small agglomeration, the three grows randomly in arbitrary directions to form the gel.

In the percolation model, the underlying lattice is square or cubic; initially, the monomers in the solution occupy the nodes of the lattice. The monomers on these nodes can make bonds randomly with their neighbors and the bond content increases steadily after the initiation. In experimental work, the sol–gel transition process is initiated by introducing special molecules called ''initiators.''

In both models, the proportion of bonds between the monomers is a characteristic of the transition process denoted as the ''bond content probability p.'' There is a threshold value for this bond content, denoted by p_c; below which the monomers form isolated

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clusters and above which infinite clusters start to form in the thermodynamic limit. This situation is characterized either by the amount of free monomers (equivalently, the gel fraction or bond content) or by the time at which this situation occurs and it is called the ''gel point.''

The proportion of monomers that have made bonds but that form isolated clusters is called ''the weight average degree of polymerization,'' and denoted by DP_w, and the proportion of monomers that make part of the infinite lattice is called the ''gel fraction'' and denoted by G. As time passes, the isolated clusters merge to the gel component.

The behavior of the phase transition near the gel point is different for the classical and the percolation models. Near the gel point, ''the weight average degree of polymerization,'' DP_w and the ''gel fraction'' G behave as

$$DP_w \propto (p_c - p)^{-\gamma} \quad p \to p_c^- \tag{1}$$

$$G \propto (p - p_c)^{\beta} \quad p \to p_c^+ \tag{2}$$

The Flory–Stockmayer (classical) theory gives $\beta = \gamma = 1$, independent of the dimensionality while the percolation studies based on computer simulations give γ and β around 1.7 and 0.43 in three-dimension [6,7].

In experimental work on sol–gel transitions, it has been observed that, depending on the values of the parameters, the same system may exhibit properties that correspond to either of these models [8–10]. In order to decide which model applies, the gel point is determined (usually) experimentally and the log–log plots around the gel point are computed with necessary corrections in order to see which theory fits best to the observed behavior around the gel point.

The sol–gel transition for polyacrylamide (PAAm)–sodium alginate (SA) composite with different concentrations of SA has been studied in Evingür et al. [8], where it is shown that the phase transitions for composites with low SA concentrations obey the percolation model, while for high SA concentrations the Flory–Stockmayer theory is more appropriate. The phase transition curves for different SA concentrations in classical and percolation type phase transitions are shown in Figures 1 and 2, respectively.

In our study, we have applied two well-known models of epidemiology, the ''Susceptible-Infected-Removed'' (SIR) and ''Susceptible-Exposed-Infected-Removed'' (SEIR) epidemic models to the phase transitions of PAAm–SA composite. We describe below the general features of these models and present their detailed discussion in Section 2.

The spread of epidemics in a population is described by the so-called compartmental models. In these models, the individuals in the population are initially in disjoint compartments. The people who have no immunity are in the ''susceptible'' (S) compartment. The infectious agent may or may not have a latent period. If there is no latent period, the individuals show symptoms as soon as they get the virus and contaminate it to the individuals they contact. The ''infected'' (I) individuals recover (or die) after a certain period characteristic of the disease. At any rate, they move into the compartment denoted as ''recovered'' or ''removed'' (R) [11]. This simple model is called the SIR epidemic model. If the infectious agent has a latent period, then the individuals that get in contact with the virus first move into the ''exposed'' (E) department where they show no symptoms. After an incubation period which is a characteristic of the disease, the exposed individuals move into the ''infected'' (I) and then into the ''removed''

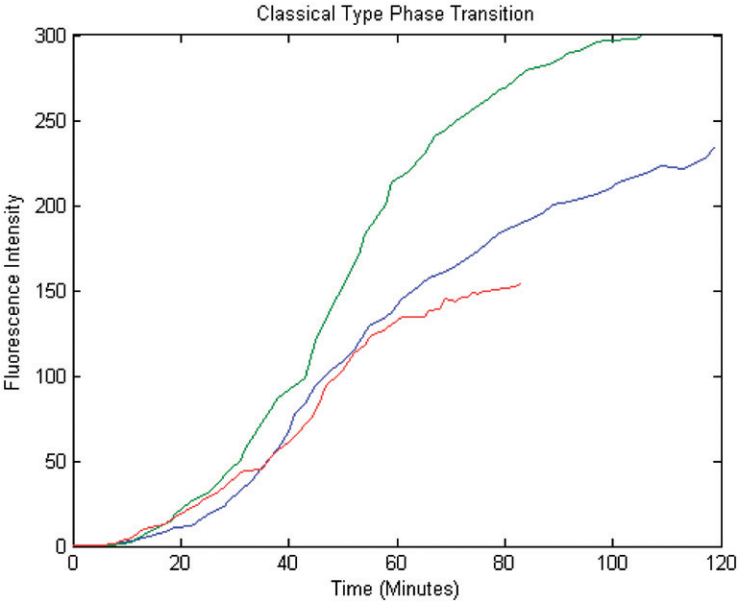

Figure 1. Experimental data for classical type phase transition for PAAm–SA composite obtained by fluorescence measurements. The SA concentrations are 1.50%, 1.00%, and 0.50% (w/v). Higher SA concentrations slow down the reaction and lead to slower rise of the gel fraction [8].

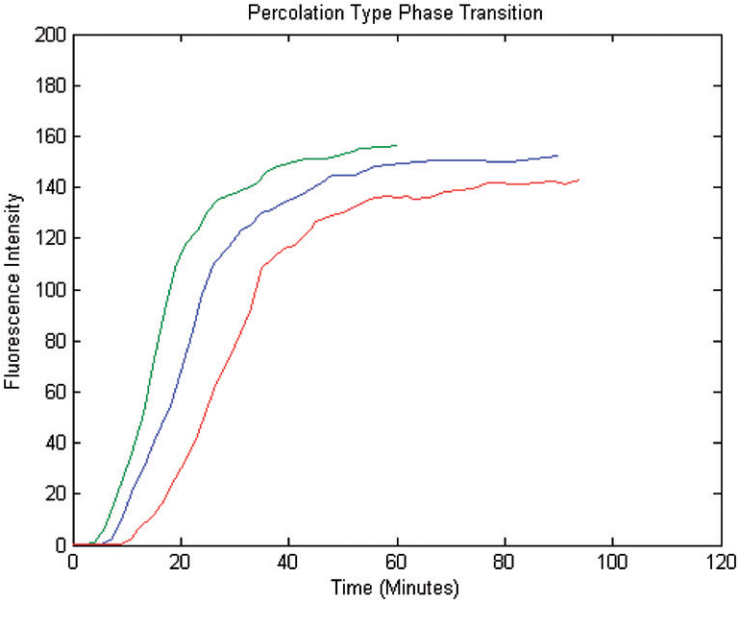

Figure 2. Experimental data for percolation type phase transition for PAAm–SA composite obtained by fluorescence measurements. The SA concentrations are 0.25%, 0.12%, and 0.06% (w/v). Lower SA concentrations result in faster reactions and lead to faster rise of the gel fraction [8].

(R) compartments. This model including the incubation stage is called the SEIR epidemic model.

In both the SIR and SEIR models, the number of "removed" individuals (R) raises monotonically from zero to a steady-state value R_f. The monotone passage between two stable states in the time domain is suggestive for using the SIR and SEIR models for phase transitions. On the other hand, the interactions of the individuals and the mechanism for the spread of an epidemic are modeled on networks [11–13]. In this article, we have solved the differential equations for the SIR and SEIR models over a wide range of parameters and compared the experimental and theoretical results to determine the best model and parameter values that fit the observed phase transitions. We have seen that the "SIR" epidemic model was appropriate for the group of experiments that were labeled as to fit the percolation model. On the other hand, the classical type phase transition could not be modeled by the SIR model, but they fit well the "SEIR" epidemic model solutions.

The SIR and SEIR models are described, respectively, in Sections 2.1 and 2.2, the exact solution of the SIR model is given in Section 2.3, and the models for the experimental data are presented in Section 3.

2. Epidemic models and phase transitions

2.1. *The SIR and the model*

In the SIR model, the individuals in a society are in the "susceptible (S)," "infected (I)," and "recovered (R)" states and only one-directional passages among states are allowed. A person who has no immunity is in the group of susceptible individuals. Susceptible individuals are infected as a result of interaction with infected individuals. The rate of change of the susceptible individuals is proportional to the product of susceptible and infected individuals. This proportionality constant and the duration of the infectious period are characteristics of the disease. Since the passage among states is one directional, infected individuals gain immunity at the end of the infectious period and move into the removed compartment. In the simplest case, the total number of individuals in the population and the parameters of the model are constant. This model is suitable for the description of short-term epidemics in a closed society. The differential equations that govern this model are given below:

$$\mathrm{d}S/\mathrm{d}t = -k\,I(t)S(t) \tag{3}$$

$$\mathrm{d}I/\mathrm{d}t = k\,I(t)\,S(t) - \eta I(t) \tag{4}$$

$$\mathrm{d}R/\mathrm{d}t = \eta I(t) \tag{5}$$

The subsystem consisting of the nonlinear coupled equations for S and I describes the dynamics of the model. Once these are solved, R can be obtained by a quadrature. In this model, the inverse of the parameter η is related to the duration of the infectious period. Thus, smaller value of the parameter η corresponds to longer infectious periods. In this dynamical system, the parameter η can be set equal to 1 by a scaling of time and the dynamical properties of the system depend only on the ratio η/k. In particular, the final value of R, depends on η/k only.

The number of susceptible and removed individuals in the SIR and SEIR models can be thought of, respectively, as the initial and final products in a phase transition. The role of the infected individuals is played by the components that mediate the transition process.

In the case of the transition from the sol to the gel state, the bulk of molecules in the phase transition experiment constitute the analog of the population. The set of monomers that are susceptible to make bonds play the role of "susceptible" individuals, while the molecules that already made bonds and can no longer react, play the role of the "removed" individuals. The mechanism of the transition form the sol to the gel state is through the molecules that play the role of "infected" individuals. This transition is realized through the production of monomers with free radicals that make bonds with other monomers to form chains, small clusters or a network.

We should note that the SIR and SEIR models are insensitive to the detailed structure of the transition mechanism. These models are determined by two and three parameters, respectively, hence, if they really represent the mechanism of the phase transition, there should be some set of parameters for which theoretical and experimental results agree.

Since the final gel fraction is a function of the ratio η/k, the parameters are chosen in a range that would lead to reasonably high final gel fractions that are characteristic of these experiments. We have seen that low values of η/k give rise to sharper transition curves that are characteristic of the phase transitions of percolation type. The smoother rise that is characteristic of the classical phase transition can be obtained by η/k values close to 1 [14]. As it will be discussed in Section 3, the normalized transition curves for classical type phase transitions may be approximated by SIR model normalized transition curves with η/k close to 1, but the final gel fractions are too small to represent gel formation hence the SEIR model is needed to model phase transitions of classical type.

2.2. *The SEIR and the model*

The SEIR model refers to the differential equations governing the dynamics of a population where the individuals can be "susceptible (S)," "exposed (E)," "infected (I)," and "removed (R)" and only one-directional passages among states are allowed. A person who has no immunity is in the group of susceptible individuals. Susceptible individuals first become "exposed" when they have the virus but they do not show symptoms. Then after an incubation period, they start showing the symptoms and contaminate other people. Here also immunity cannot be lost and the total number of individuals in the population and the parameters of the model are constant. The differential equations are modified as follows.

$$\mathrm{d}S/\mathrm{d}t = -kI(t)S(t) \tag{6}$$

$$\mathrm{d}E/\mathrm{d}t = kI(t)S(t) - \varepsilon E(t) \tag{7}$$

$$\mathrm{d}I/\mathrm{d}t = \varepsilon E(t) - \eta I(t) \tag{8}$$

$$\mathrm{d}R/\mathrm{d}t = \eta I(t) \tag{9}$$

As it will be seen in the next section, in this model also, the final gel fraction R_f depends on η/k only. But here the existence of the latent period leads to smoother transition curves even for low values of η/k. Thus, the SEIR model can represent classical phase transitions that end with a high gel fraction *via* a smoother rise.

2.3. *Exact solution of the dynamical system*

In the SIR model as a dynamical system, the (S, I) system (3) and (4) can be solved exactly by a sequence of elementary integrations. For this, we first find the derivative of I with respect to S. Using the chain rule, we have $\mathrm{d}I/\mathrm{d}t = \mathrm{d}I/\mathrm{d}S\ \mathrm{d}S/\mathrm{d}t$.

Hence

$$\mathrm{d}I/\mathrm{d}S = (kSI - \eta I)/(-kSI) = -1 + 1/S \tag{10}$$

This equation can be integrated easily and using the initial conditions $S(t_0) = S_0$, $I(t_0) = I_0 = 1 - S_0$, we have

$$I(S) = 1 - S + (\eta/k)\ln(S/S_0) \tag{11}$$

Similarly one can see that $R = -(\eta/k)\ \ln(S/S_0)$, but this relation is not useful. Instead, we need the fact that at the steady state $I = 0$; hence, the steady-state value of S, S_f is given by the solution of the transcendental equation

$$0 = 1 - S_f + (\eta/k)\ln(S_f/S_0) \tag{12}$$

The final value of the gel fraction is

$$R_f = 1 - S_f \tag{13}$$

In the SEIR model, $E + I$ satisfies the same equation as I in the SIR model. In this model, the steady state is characterized by $I = E = 0$, hence the final values of S and R are given by Equations (12) and (13), thus, the final gel fraction in both models is determined by the initial value S_0 and the ratio (η/k). In the sol–gel transition experiments, it is known that the final gel fraction is high; hence in either model, we expect the parameter η/k to be low.

Finally, we note that the SIR model can be thought of as a special case of the SEIR model where the incubation period is zero; i.e., the parameter ε is infinity. Thus, if a phase transition can be modeled by the SIR model, we will be content with it and would not search for a SEIR model for this transition.

3. The model parameters

We have solved the SIR and SEIR models for a wide range of system parameters and initial conditions, and compared with the experimental data. In doing this, we have started with a coarse grid and looked for solutions that result in at least 80%, final gel fraction. We have found localizations of the low error regions and scanned these areas of the parameter space more finely.

We have seen that the percolation type phase transitions can be modeled by the SIR model with a final gel fraction of at least 90%. The normalized phase transition curves of classical type could be approximated by a SIR model with η/k close to 1, but in this case the final gel fraction was very low, hence, we concluded that the SIR model could not represent phase transitions of classical type. The classical type phase transitions are then modeled with the SEIR system.

The parameters given below correspond to the models with lowest errors. In some cases, there are more than one model with best fit, these models are close to each other, we have chosen the ones that qualitatively fit better. The model parameters are given in Tables 1 and 2, and selected graphs are presented in Figures 3 and 4.

Table 1. Parameters for the SEIR model for classical phase transition.

Concentration	1.50	1.00	0.50
k	0.5025	0.2450	0.1780
ε	0.1000	0.1600	0.200
η	0.1500	0.0500	0.0400
η/k	0.2985	0.2041	0.2247
I_0	$10^{-1.50}$	$10^{-1.40}$	$10^{-1.25}$
R_f	0.9172	0.9696	0.9394
Error (%)	4.05	2.42	4.42

Table 2. Parameters for the SIR model for percolation type phase transition.

Concentration	0.25	0.12	0.06
k	0.3780	0.6360	0.4600
η	0.0900	0.1200	0.1000
η/k	0.2381	0.1887	0.2174
I_0	$10^{-2.40}$	$10^{-2.05}$	$10^{-2.02}$
R_f	0.9820	0.9920	0.9889
Error (%)	2.07	2.27	2.59

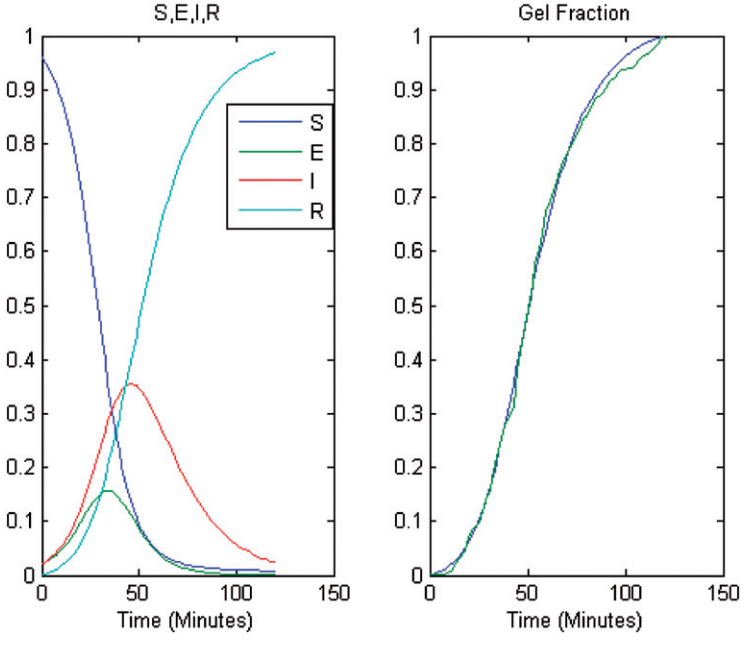

Figure 3. (a) Solution curves for the SEIR model with parameters, $k = 0.2450$, $\varepsilon = 0.1600$, $\eta = 0.0500$, $\eta/k = 0.2041$, and initial value $I_0 = 10^{-1.40}$. Final value of the gel fraction is 0.9696 and (b) comparison of the normalized gel fractions for the experimental result for AL 1.00%(w/v) concentration and the SEIR model normalized $R(t)$. The least squares error is 2.42%.

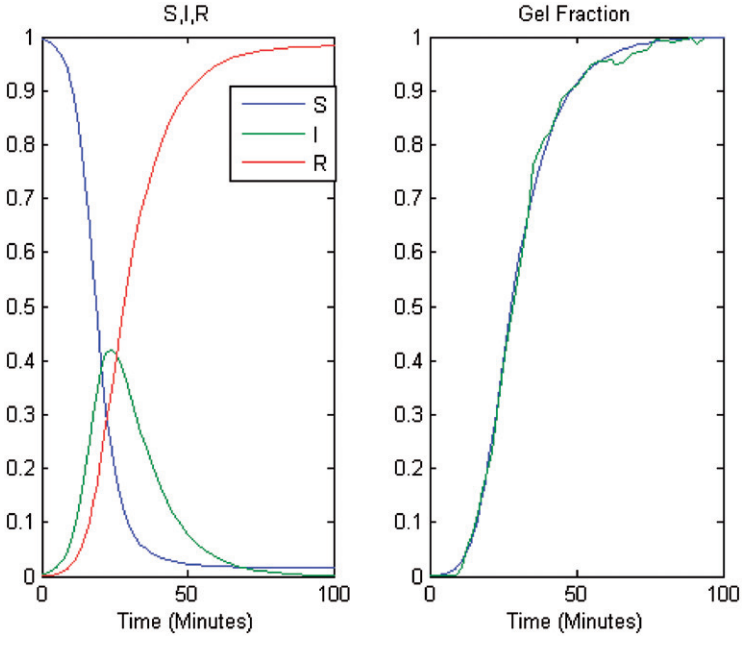

Figure 4. (a) Solution curves for the SIR model with parameters, $k = 0.3780$, $\eta = 0.0900$, $\eta/k = 0.2381$, and initial value $I_0 = 10^{-2.40}$. Final value of the gel fraction is 0.9820 and (b) comparison of the normalized gel fractions for the experimental result for AL 0.25%(w/v) concentration and the SIR model normalized $R(t)$. The least squares error is 2.07%.

4. Conclusions

From here, we conclude that the spread of epidemics can be modeled using the percolation and classical pictures which are well-established models in phase transition phenomenon. In this study, it has been shown that SEIR and SIR models fit to the classical and the percolation type phase transition models, respectively.

References

[1] P.J. Flory, *Molecular size distribution in three dimensional polymers. I. Gelation*, J. Am. Chem. Soc. 63 (1941), pp. 3083–3090.
[2] P.J. Flory, *Molecular size distribution in three dimensional polymers. II. Trifunctional branching units*, J. Am. Chem. Soc. 63 (1941), pp. 3091–3096.
[3] P.J. Flory, *Molecular size distribution in three dimensional polymers. III. Tetrafunctional branching units*, J. Am. Chem. Soc. 63 (1941), pp. 3096–3100.
[4] W. Stockmayer, *Theory of molecular size distribution and gel formation in branched-chain polymers*, J. Chem. Phys. 11 (1943), pp. 45–54.
[5] W. Stockmayer, *Theory of molecular size distribution and gel formation in branched polymers II. General cross linking*, J. Chem. Phys. 12 (1944), pp. 125–129.
[6] D. Stauffer, A. Coniglio, and M. Adam, *Gelation and critical phenomena*, Adv. Polym. Sci. 44 (1982), pp. 103–158.
[7] D. Stauffer and A. Aharony, *Introduction to Percolation Theory*, 2nd ed., Taylor and Francis, London, 1994.

[8] G.A. Evingür, F. Tezcan, F.B. Erim, and Ö. Pekcan, *Monitoring the gelation of polyacrylamide-sodium alginate composite by fluorescence technique*, Phase Transitions. Available at http://dx.doi.org//10.1080/01411594.2011.629363 (in press)
[9] D. Kaya, O. Pekcan, and Y. Yilmaz, *Direct test of the critical exponents at the sol-gel transition*, Phys. Rev. E: Stat. Nonlinear Soft Matter Phys. 69 (2004), Article number 016117 (1–10).
[10] D. Kaya Aktaş, G. Akın Evingür, and Ö. Pekcan, *Universal behaviour of the gel formation from Acrylamide-carrageenan mixture around the gel point: A fluorescence study*, J. Biomol. Struct. Dyn. 24(1) (2006), pp. 83–90.
[11] H.W. Hethcote, *The mathematics of infectious diseases*, SIAM Rev. 42 (2000), pp. 599–653.
[12] M.E.J. Newman, *Spread of epidemics on networks*, Phys. Rev. E: Stat. Nonlin. Soft Matter Phys. 66 (2002), Article number 016128 (1–8).
[13] Y. Yılmaz, A. Erzan, and Ö. Pekcan, *Critical exponents and fractal dimension at the sol-gel phase transition via in situ fluorescence experiments*, Phys. Rev. E: Stat. Nonlin. Soft Matter Phys. 58 (1998), pp. 7487–7491.
[14] D.R. de Souza, T. Tomé, and R.M. Ziff, *A new scale-invariant ratio and finite-size scaling of the stochastic susceptible-infected-recovered model*, J. Stat. Mech.: Theory Exp. (2011), Article number p03006 (1–12).