Pattern formation simulations in reaction-diffusion systems by Local Integral Equation method with Meshless approximations

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Outline of the presentation

- Turing systems
- Mathematical formulation of reaction-diffusion problems
- Local integral equation formulation ; discretization
- Numerical examples
1. Turing systems

- It is well known a **homogenizing** influence of diffusion in nature.
- Alan Turing discovered [1]: **spatial patterns would be formed by a reaction-diffusion system combining local activation with long range inhibition**


Turing also pointed out the role of such patterns in **biological pattern formation**.

The spots of a cheetah can be imitated by using a Turing model.
A typical Turing system is a **reaction-diffusion system** consisting of at least two chemical species (activator and inhibitor) exhibiting a steady state which is stable to small perturbations in the absence of diffusion, but becomes unstable when **diffusion is present** (Turing instability).

The formation of spatial patterns is principally a **nonlinear phenomenon**. Otherwise the unstable modes would grow unlimitedly.

Linear theory does **determine conditions under which spontaneous pattern formation is allowed for certain parameter ranges**.

Initial and boundary conditions, the shape and size of the domain yield various forms of patterns. **To determine which of the various possible patterns will be stable or which conversion takes place, one has to go beyond linear theory.**
Various numerical methods have been used to solution of nonlinear reaction-diffusion systems and computer simulations of pattern formation.

In this paper, we developed the **Local integral equation (LIE) method** for numerical simulations of 2-d pattern formation in reaction-diffusion systems.

- truly meshless formulation (element-free formulation)
- MLS approximation for spatial variation of field variables
- time discretization by using one-step $\theta$-method
- LIE – weak formulation of the differential governing equations on local sub-domains considered around each interior node with using the Green function of the Laplace operator as the test function
- circular shape of sub-domains → possibility to find the Green function vanishing on the boundary of the sub-domain and so eliminate the normal derivatives of the field variables from the formulation ⇒ better accuracy and savings of computational time (derivatives are eliminated)
- the nonlinear terms are treated iteratively within each time step
2. Mathematical formulation of reaction-diffusion problems

- **Governing equations** for the concentrations of two chemicals \( u(x,t) \) and \( v(x,t) \) subjected to reaction-diffusion processes [J.D. Murray: *Mathematical Biology, Springer-Verlag, Berlin, 2003]*

\[
\frac{\partial u}{\partial t} = \nabla^2 u + \gamma f(u,v), \quad \frac{\partial v}{\partial t} = d \nabla^2 v + \gamma g(u,v) \quad \text{in } \Omega \times [0,T]
\]

- **initial values** \( \{u(x,0), v(x,0)\} \)

- **boundary conditions** (usually taken as the Neumann type): \[
\frac{\partial u}{\partial n} = 0, \quad \frac{\partial v}{\partial n} = 0 \quad \text{on } \partial \Omega
\]

(no external input)
• **homogeneous steady state** \((u_0,v_0)\) is the positive solution of \(f(u,v)=0\), \(g(u,v)=0\)

• **linearized** reaction-diffusion system

\[
\frac{\partial w}{\partial t} = D\nabla^2 w + \gamma A w, \quad D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}, \quad w = \begin{pmatrix} u-u_0 \\ v-v_0 \end{pmatrix}, \quad A = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix}
\]

expansion of the solution

\[
w(x,t) = \sum_k c_k e^{\omega t} W_k(x),
\]

\(W_k(x)\) - eigenfunction of the Laplace operator corresponding to the eigenvalue \(k^2\)

\(\omega(k^2)\) determines temporal growth of the linearized solution and it is determined by the roots of the characteristic equation

\[
\omega^2 + \omega \left[ k^2(1+d) - \gamma(f_u + g_v) \right] + h(k^2) = 0 \quad \text{with} \quad h(k^2) = k^4d - k^2\gamma(df_u + g_v) + \gamma^2(f_ug_v - f_vg_u)
\]
• **linear stability** of the homogeneous $[\nabla(.) \equiv 0, k^2=0]$ steady state solution yields constraints

$$f_{,u} + g_{,v} < 0, \quad f_{,ug,v} - f_{,vg,u} > 0.$$ 

• for **diffusion-driven instability** of steady state solution to spatial disturbances we require

$$\text{Re}\omega(k^2) > 0 \quad \text{for some} \quad k^2 \neq 0$$

this can happen only if $h(k^2) < 0$ for some $k^2 \neq 0$

$$\Rightarrow \text{additional necessary conditions for the generation of spatial patterns (with } k^2 \neq 0):$$

$$ (df_{,u} + g_{,v}) > 0, \quad (df_{,u} + g_{,v})^2 - 4d(f_{,ug,v} - f_{,vg,u}) > 0$$

$$ (\Rightarrow d \neq 1, \text{ and } f_{,ug,v} < 0)$$
- An **analysis of the dispersion relation** \( \omega = \omega(k^2) \) says which eigenfunctions, i.e. which spatial patterns are linearly unstable and grow exponentially with time \( \text{Re} \omega(k^2) > 0 \)

  (in finite domain eigenvalue problems, the wavenumbers are discrete)

- In nonlinear RD problems there are mechanisms which do not allow unbounded growth of unstable modes with \( t \to \infty \).

- Therefore the **linear stability analysis** (though informative) is not complete for post buckling evolution and it is necessary to know the **solution of the nonlinear problems** with taking into account the prescribed boundary and initial conditions as well as the geometry of the analyzed domain.
3. Local integral equation formulation; discretization

**Weak form of the governing equations** on an arbitrary sub-domain $\Omega^s$ of the analyzed 2-d domain $\Omega$

\[
\Omega^s \left[ \frac{\partial u}{\partial t} - \nabla^2 u - \gamma f(u,v) \right] u^* dx = 0 , \quad \Omega^s \left[ \frac{\partial v}{\partial t} - d \nabla^2 v - \gamma g(u,v) \right] u^* dx = 0 , \quad u^* - \text{test function}
\]

appropriate choice: **Green function** of the Laplace operator

\[
u^*(r) = -\frac{1}{2\pi} \ln \left( \frac{r}{r_0} \right) , \quad u^*(r) \bigg|_{\partial \Omega^c} = 0 , \quad r = r = \|x - x^c\| \]

sub-domain $\Omega^c$ - a circle of the radius $r_0$ and centered at the point $x^c \in \Omega$

\[
\downarrow
\]
LIE: \[ u(x^c,t) + \int_{\partial \Omega^c} u(x,t) \frac{\partial u^*(x-x^c)}{\partial n(x)} d\Gamma + \int_{\Omega^c} \left[ \frac{\partial u(x,t)}{\partial t} - \gamma f(u(x,t),v(x,t)) \right] u^*(x-x^c) d\Omega = 0 \]

\[ dv(x^c,t) + d \int_{\partial \Omega^c} v(x,t) \frac{\partial v^*(x-x^c)}{\partial n(x)} d\Gamma + \int_{\Omega^c} \left[ \frac{\partial v(x,t)}{\partial t} - \gamma g(u(x,t),v(x,t)) \right] u^*(x-x^c) d\Omega = 0 \]

normal derivatives \( \frac{\partial u(x,t)}{\partial n} \), \( \frac{\partial v(x,t)}{\partial n} \) are not involved in LIE

**MLS-approximation** for spatial variations of the field variable \( w(x,t) \in \{u(x,t), v(x,t)\} \):

\[ w(x,t) \approx \hat{w}(x,t) = \sum_{a=1}^{n} \hat{\omega}^a(t) \phi^a(x) \quad \phi^a(x) \text{ - shape function associated with the node } x^a \]

\( \hat{\omega}^a(t) \neq w(x^a,t) \) - nodal unknown

Gaussian weights
Semi-discretized LIE + b.c. (ODE for unknowns \{\hat{u}^a(t), \hat{v}^a(t)\}, a=1,2,...,n) :

\[
\sum_{a=1}^{n} \frac{\partial \hat{u}^a(t)}{\partial t} A^{ca} + \sum_{a=1}^{n} \hat{u}^a(t) B^{ca} - \gamma \int_{\Omega^c} f(\bar{u}(x,t),\bar{v}(x,t)) u^*\left(\|x-x^c\|\right) d\Omega = 0, \quad x^c \in \Omega \quad \text{LIE}
\]

\[
\sum_{a=1}^{n} \frac{\partial \hat{v}^a(t)}{\partial t} A^{ca} + d \sum_{a=1}^{n} \hat{v}^a(t) B^{ca} - \gamma \int_{\Omega^c} g(\bar{u}(x,t),\bar{v}(x,t)) u^*\left(\|x-x^c\|\right) d\Omega = 0, \quad x^c \in \Omega \quad \text{LIE}
\]

\[
\sum_{a=1}^{n} \hat{u}^a(t) D^{ba} = 0, \quad \sum_{a=1}^{n} \hat{v}^a(t) D^{ba} = 0, \quad x^b \in \partial \Omega, \quad \text{b.c.}
\]

where \[ A^{ca} = \int_{\Omega^c} \phi^a(x) u^*\left(\|x-x^c\|\right) d\Omega, \quad B^{ca} = \phi^a(x^c) + \int_{\partial \Omega^c} \phi^a(x) \frac{\partial u^*\left(\|x-x^c\|\right)}{\partial n(x)} d\Gamma, \quad D^{ba} = \frac{\partial \phi^a}{\partial n}(x^b) \]
Approximate integrations

boundary integrals

\[ C^{ca} := \int_{\partial \Omega^c} \phi^a(x) \frac{\partial u^*}{\partial n(x)} d\Gamma = \frac{1}{2\pi} \int_0^{2\pi} \phi^a(x_1^c + r_0 \cos \phi, x_2^c + r_0 \sin \phi) d\phi = \]

\[ = \frac{1}{2} \int_{-1}^1 \phi^a \left( x_1^c + r_0 \cos \pi(1+s), x_2^c + r_0 \sin \pi(1+s) \right) ds = \]

\[ \approx \frac{1}{2} \sum_{g=1}^N w^g \phi^a \left( x_1^c + r_0 \cos \pi(1+s_g), x_2^c + r_0 \sin \pi(1+s_g) \right), \quad \text{Gauss-Legendre quadrature rule} \]

\[ B^{ca} \approx \phi^a(x^c) + C^{ca} \]

domain integrals

\[ \int_{\Omega^c} h(x) u^* \left( \|x - x^c\| \right) d\Omega = \int_{\Omega^c} \left[ h(x^c) + h_x(x^c)(x - x^c) + h_y(x^c)(y - y^c) + \ldots \right] u^* \left( \|x - x^c\| \right) d\Omega = \]

\[ = \frac{h(x^c)}{2\pi} \int_0^{2\pi} d\phi \int_0^r \frac{r_0}{r} dr - \frac{1}{2\pi} \left[ h_x(x^c) \int_0^{2\pi} \cos \phi d\phi + h_y(x^c) \int_0^{2\pi} \sin \phi d\phi \right] \int_0^r r_0 \ln \frac{r_0}{r} dr + O \left( r_0^4 \right) = \]
\[-h(x^c) \int_0^{r_0} r \ln \frac{r}{r_0} \, dr + O\left(\frac{r_0^4}{r_0}\right) = \left(\frac{r_0}{2}\right)^2 h(x^c) + O\left(\frac{r_0^4}{r_0}\right)\]

Assuming the radius of sub-domains to be sufficiently small, one can neglect the terms \(O\left(\frac{r_0^4}{r_0}\right)\). Thus,

\[
A^{ca} \approx \left(\frac{r_0}{2}\right)^2 \phi^{a}(x^c), \quad \int_{\Omega^c} f\left(\bar{u}(x,t), \bar{v}(x,t)\right) u^{*}\left(\|x-x^c\|\right) \, d\Omega \approx \left(\frac{r_0}{2}\right)^2 f\left(\bar{u}(x^c,t), \bar{v}(x^c,t)\right)
\]

\[
\int_{\Omega^c} g\left(\bar{u}(x,t), \bar{v}(x,t)\right) u^{*}\left(\|x-x^c\|\right) \, d\Omega \approx \left(\frac{r_0}{2}\right)^2 g\left(\bar{u}(x^c,t), \bar{v}(x^c,t)\right)
\]

(saving computational time)
Now, the system of the non-linear ODE becomes

\[
\begin{pmatrix}
M \frac{\partial}{\partial t} + K & 0 \\
0 & M \frac{\partial}{\partial t} + dK
\end{pmatrix}
\begin{bmatrix}
\hat{U} \\
\hat{V}
\end{bmatrix}
- \begin{bmatrix}
F \\
G
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix},
\]

where \( M, K \) are \((n\times n)\) matrices,

\[
M^{da} = \begin{cases}
A^{da}, & x^d \in \Omega \\
0, & x^d \in \partial \Omega
\end{cases}, \quad K^{da} = \begin{cases}
B^{da}, & x^d \in \Omega \\
D^{da}, & x^d \in \partial \Omega
\end{cases}, \quad (d, a=1, 2, \ldots, n)
\]

\[
\hat{U} = \begin{bmatrix}
\hat{u}^1(t), \ldots, \hat{u}^n(t)
\end{bmatrix}^T, \quad \hat{V} = \begin{bmatrix}
\hat{v}^1(t), \ldots, \hat{v}^n(t)
\end{bmatrix}^T, \quad F = \begin{bmatrix}
F^1, \ldots, F^n
\end{bmatrix}^T, \quad G = \begin{bmatrix}
G^1, \ldots, G^n
\end{bmatrix}^T,
\]

\[
F^d = \gamma \left( \frac{r_0}{2} \right)^2 \begin{cases}
f(\bar{u}(x^d, t), \bar{v}(x^d, t), x^d \in \Omega) \\
0, & x^d \in \partial \Omega
\end{cases}, \quad G^d = \gamma \left( \frac{r_0}{2} \right)^2 \begin{cases}
g(\bar{u}(x^d, t), \bar{v}(x^d, t), x^d \in \Omega) \\
0, & x^d \in \partial \Omega
\end{cases}.
\]
Time discretization

\[ \theta \text{-method : } \quad \frac{\partial w}{\partial t} = \Phi(w(t)) \quad \theta = 1 \text{ Euler m. (explicit, conditionally stable); } \theta \in [0,1) \text{ - implicit m., unconditionally stable} \]

\[ \frac{\partial \hat{w}^a}{\partial t} \approx \frac{\hat{w}^a_{k+1} - \hat{w}^a_k}{\Delta t} = \theta \Phi(\hat{w}^a_{k+1}) + (1-\theta)\Phi(\hat{w}^a_k), \quad \hat{w}^a_k = \hat{w}^a(t_k) \in \{\hat{u}^a(t_k), \hat{v}^a(t_k)\}, \quad 0 \leq \theta \leq 1, \quad \theta = 1/2 \]

System of nonlinear algebraic equations for 2n unknowns \{\hat{u}^a_{k+1}, \hat{v}^a_{k+1}\}, (a=1,...,n)

\[ \begin{bmatrix} M + \theta \Delta t K & 0 \\ 0 & M + d \theta \Delta t K \end{bmatrix} \begin{bmatrix} \hat{U}_{k+1} \\ \hat{V}_{k+1} \end{bmatrix} - \theta \Delta t \begin{bmatrix} F_{k+1} \\ G_{k+1} \end{bmatrix} = \begin{bmatrix} M - (1-\theta)\Delta t K & 0 \\ 0 & M - d(1-\theta)\Delta t K \end{bmatrix} \begin{bmatrix} \hat{U}_k \\ \hat{V}_k \end{bmatrix} + (1-\theta)\Delta t \begin{bmatrix} F_k \\ G_k \end{bmatrix}, \text{ solved subsequently for } (k=0,1,...,F) \]

The initial values \( \hat{w}^a_0 \):

\[ \sum_{a=1}^{n} \hat{w}^a_0 \phi^a(x^c) = w(x^c,0), \quad (c=1,...,n). \]

The nonlinearities are involved in \( F \) and \( G \) terms (iterative solution).
4. Numerical examples

**Schnakenberg model** is one of the most interesting Turing models in pattern formation.

**Dimensional form** of the model

\[
\frac{\partial A}{\partial t} = d_A \nabla^2 A + k_1 - k_2 A + k_3 A^2 B, \quad \frac{\partial B}{\partial t} = d_B \nabla^2 B + k_4 - k_3 A^2 B
\]

* A and B are concentrations of two chemical species with diffusion rates \(d_A\) and \(d_B\).
* \(k_i\)'s are the positive rate constants.

**Rescaling**

\[
A = \sqrt{\frac{k_3}{k_2}}, \quad B = \sqrt{\frac{k_3}{k_2}}, \quad t^* = \frac{d_A t}{L^2}, \quad x^* = \frac{x}{L}, \quad a = \frac{k_1}{k_2}, \quad b = \frac{k_4}{k_2}, \quad d = \frac{d_B}{d_A}, \quad \gamma = \frac{L^2 k_2}{d_A}
\]

**Dimensionless RD system** (dropping the asterisks for algebraic convenience)

\[
\frac{\partial u}{\partial t} = \nabla^2 u + \gamma \left(a - u + u^2 v\right), \quad \frac{\partial v}{\partial t} = d \nabla^2 v + \gamma \left(b - u^2 v\right)
\]

which is a special case of Turing system with \(f = a - u + u^2 v\), \(g = b - u^2 v\).
The uniform positive steady state \((u_0, v_0)\):

\[
\begin{align*}
u_0 &= a + b, \\
v_0 &= \frac{b}{(a+b)^2}, \quad b > 0, \quad a+b>0
\end{align*}
\]

hence

\[
\begin{align*}
f_{,u} &= \frac{b-a}{b+a}, \\
f_{,v} &= (b+a)^2 > 0, \\
g_{,u} &= \frac{-2b}{b+a} > 0, \\
g_{,v} &= -(b+a)^2 < 0.
\end{align*}
\]

The necessary conditions for pattern formation

\[
\begin{align*}
f_{,u} + g_{,v} < 0 & \quad \Rightarrow \quad 0 < b - a < (a+b)^3 \\
f_{,u} g_{,v} - f_{,v} g_{,u} > 0 & \quad \Rightarrow \quad (a+b)^2 > 0 \\
df_{,u} + g_{,v} > 0 & \quad \Rightarrow \quad d(b-a) > (a+b)^3 \\
(df_{,u} + g_{,v})^2 - 4d(f_{,u} g_{,v} - f_{,v} g_{,u}) > 0 & \quad \Rightarrow \quad \left[ d(b-a) - (a+b)^2 \right]^2 > 4d(a+b)^4
\end{align*}
\]

**Pattern formation space** (or Turing space) = a domain in \((a,b,d)\) parameter space, within which the mechanisms is unstable to certain spatial disturbances of wavenumbers \(k\) determined by the boundary conditions and falling into the interval \(k_1^2 < k^2 < k_2^2\) with
\[ k_{l(2)}^2 = \frac{\gamma}{2d(a+b)} \left\{ d(b-a)-(a+b)^3 \mp \left[ d(b-a)-(a+b)^3 \right]^2 - 4d(a+b)^4 \right\}^{1/2}. \]

It can be seen that \( \gamma \sim L^2 \) is scale dependent. Thus, increasing the size of the domain yields larger limit values of the wave numbers \( k_1 \) and \( k_2 \) which results in new shorter wave lengths of allowable patterns.

In the presented examples, we shall illustrate the influence of the parameters, size and shape of the domain on the pattern formation and the shape of patterns.

- For the shape parameter in Gauss weights and radius of local subdomains, we have used fixed values \( c=0.7h \) and \( r_0=0.05h \).
- In all contour graphs, coloration is determined by a constant threshold value, \( u_s \) for \( u \) and \( v_s \) for \( v \), such that in the regions with white color, \( u<u_s \) and \( v<v_s \) while the regions where \( u>u_s \) and \( v>v_s \) are colored with green. The results confirm that the profiles of the function \( v \) are always 180\(^\circ\) out of phase to those of \( u \) and therefore only the profiles of \( u \) are presented.
Example 1.

analyzed domain $\Omega=[0,1] \times [0,1]$;

Homogeneous Neumann b.c.

initial conditions:

$$u(x,y,0)=u_0 + 10^{-3} \exp \left\{ -100 \left[ (x-1/3)^2 + (y-1/2)^2 \right] \right\}; \quad v(x,y,0)=v_0 = \frac{b}{(a+b)^2}$$

small perturbation to $u_0=a+b$

$n=26^2$ nodes; $\Delta t=0.005$; two iterations

Ex. 1.1 Choice of parameters in Turing space:

$\gamma=100; \quad a=0.1305; \quad b=0.7695; \quad d=20 \quad (D_u=0.05 \text{ and } D_v=1)$;

Fig. 1. The process of pattern formation with parameters in Example 1.1
Ex.1.2 Choice of some parameters out of Turing space \( a=0.7695; b=0.1305 \)

Fig. 2. No pattern occurs if the parameters are not in Turing space
1.3 The effect of the parameter $\gamma$

All parameters are fixed as in Ex. 1.1 and the results at $t=5s$ are presented for $\gamma \in \{10, 50, 75, 100\}$. It can be seen that increasing the parameter $\gamma$ results in shortening the lengths of allowable patterns (in increasing the wavenumbers).
\[ \gamma = 50 \]

\[ \gamma = 75 \]
Fig. 3. Results obtained with different values of $\gamma$ at time instant $t = 5$ for Example 1
1.4 The effect of initial conditions

We consider the problem with all parameters as in Ex 1.1, but initial conditions as random perturbation around steady state at each nodal point

\[ u(x,y,0) = u_0 + R \times \text{randn}(l), \quad v(x,y,0) = v_0 \quad \text{with} \quad R \in \{0.5, 0.05\} \]

The result at time instant \( t = 5 \) are shown in Fig. 4 using both the contour plots and the standard color plots.

\[ R = 0.05 \]
It can be seen from Figs. 1 and 4 that the formed patterns are the same as long as initial condition are used for which the method converges.
Example 2.

analyzed domains: $\Omega_1 = [0,1] \times [0,1]$ with $n=26^2$ nodes; $\Omega_2 = [-1,1] \times [-1,1]$ with $n=31^2$ nodes

Homogeneous Neumann b.c.

initial conditions:

$u(x,y,0) = u_0 + 0.05 \times \text{randn}(1)$, $v(x,y,0) = v_0 + 0.05 \times \text{randn}(1)$

$\Delta t = 0.005$; two iterations

Choice of parameters in Turing space:

$\gamma = 230.82$; $a = 0.1$; $b = 0.9$; $d = 8.6676$ ($D_u = 1$ and $D_v = 8.6676$);

The initial random perturbation is amplified and spreads, leading to formation of checkered patterns in both analyzed domains $\Omega_1$ and $\Omega_2$. 
$\Omega_1$
\( \Omega_2 ; \ t = 10 \)

\[ L_{(i)} = \text{characteristic linear size of the domain } \Omega_i \]
\[ L_{(2)} = 2 \times L_{(1)} \Rightarrow \gamma_{(2)} = 4 \times \gamma_{(1)} \Rightarrow \text{wavenumber}(2) = 2 \times \text{wavenumber}(1) \Rightarrow \]

\[ \Rightarrow \text{the length of allowable patterns in } \Omega_2 \text{ is 2 times shorter than that in } \Omega_1 \]
Example 3.

specifications of the problem are the same as in Ex.1, only the Dirichlet b.c. are considered instead of Neumann b.c. on the bottom and top sides of the domain, i.e.

\[ u(x,0,t) = u_s \quad u(x,1,t) = u_s \quad v(x,0,t) = v_s \quad v(x,1,t) = v_s \]

\[ \frac{\partial u}{\partial n}(0,y,t) = 0 \quad \frac{\partial u}{\partial n}(1,y,t) = 0 \quad \frac{\partial v}{\partial n}(0,y,t) = 0 \quad \frac{\partial v}{\partial n}(1,y,t) = 0 \]

Numerical experiment shows pattern formation even under changed b.c.
The results for both $u$ and $v$ at $t=5$
Comparison of patterns formed under different b.c.

\[ u, \ t=5, \ \text{Dirichlet \ & \ Neumann \ b.c.} \]

\[ u, \ t=5, \ \text{Neumann \ b.c.} \]
\( u, \quad t=5, \quad \text{Dirichlet & Neumann b.c.} \)

\( v, \quad t=5, \quad \text{Neumann b.c.} \)
Conclusions

- The **meshless LIE formulation** has been developed for simulation of **pattern formation in reaction-diffusion systems**.

- The **applicability of the method** to complex coupled problems **beyond the linear theory has been verified**.

- The derivatives of the field variables are involved only at boundary nodes where the Neumann b.c. are considered what **improves both the accuracy and computational efficiency of the formulation**.
Thank you very much for your attention!