

On the adaptive time-stepping for large-scale parabolic problems: computer simulation of heat and mass transfer in vacuum freeze-drying

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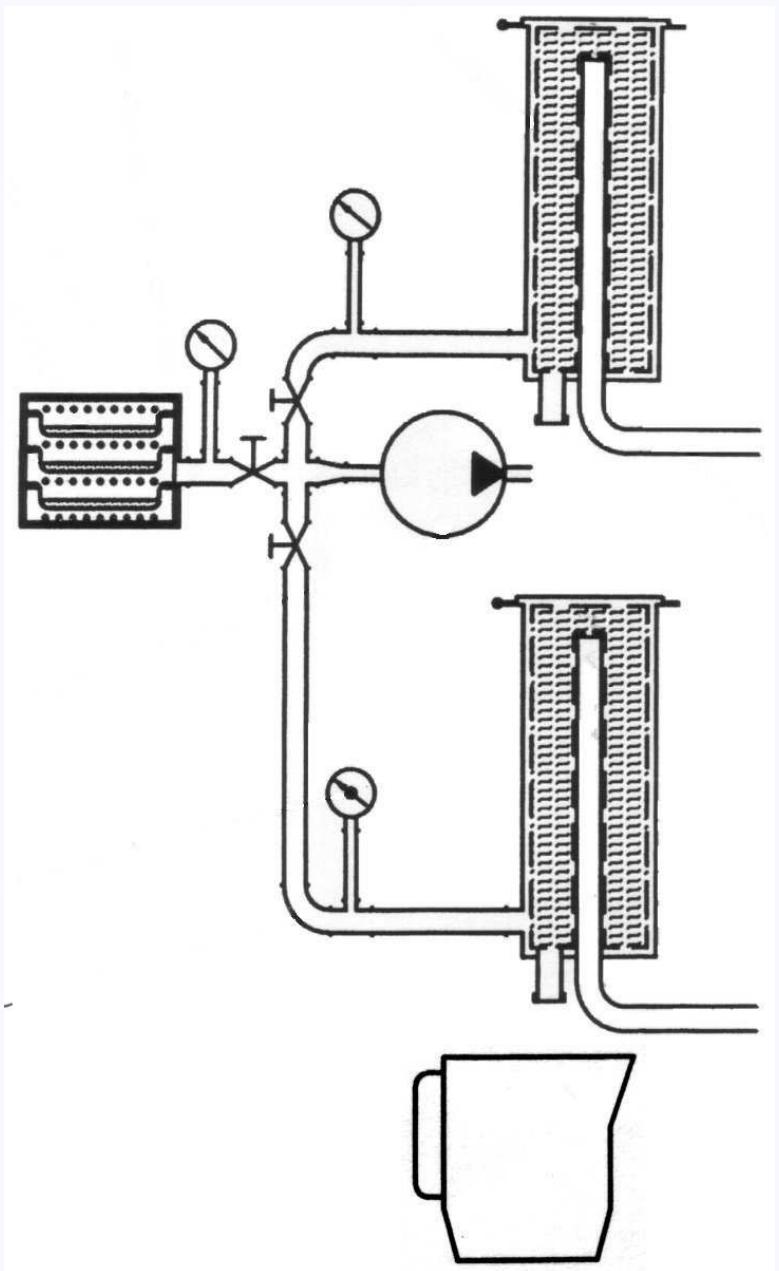
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Introduction

The work is motivated by a process of the dehydrating frozen materials by sublimation under high vacuum. The apparatus consists of two containers, one (food camera) for the product to be dried and one (absorbent camera) filled by a material (zeolite granules) for the sorbtion of water molecules.

Three phases: preparation of the source and activation (dehydration) of zeolites, self-freezing of the source, drying in conditions of an uniform sublimation of water steam.

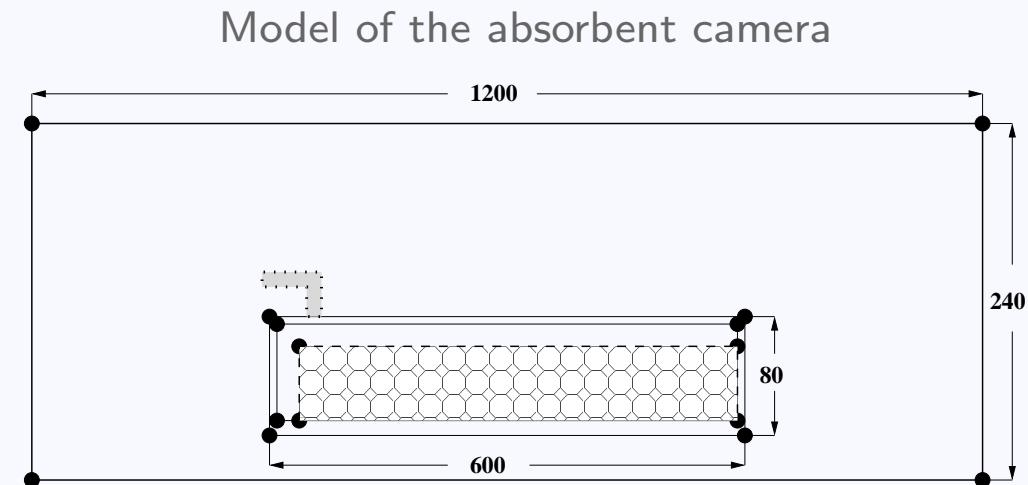
The main advantages for such kind of drying are a higher food quality of the dry due to the minimum loss of flavour and aroma, the minimal chances of the microbial to growth due to the water absence and no thermal and oxidizing processes.



Heat and mass transfer problem

$$c\rho \frac{\partial T}{\partial t} = \mathcal{L}T + f(x, t, T) \quad x \in \Omega, t > 0$$

$$\mathcal{L}T = \sum_{i=1}^d \frac{\partial}{\partial x_i} \left(k(x, t) \frac{\partial T}{\partial x_i} \right)$$



Notations:

$T(x, t)$ unknown distribution of the temperature, d dimension of the space ($d = 2$), $\Omega \in R^d$ computational domain, $k = k(x, t) > 0$ heat conductivity, $c = c(x, t) > 0$ heat capacity, $\rho > 0$ material density, $f(x, t, T)$ function responsible for the non-linear process of transfer of water molecules in the absorption container.

Initial conditions:

$$T(x, 0) = T_0(x) \quad x \in \Omega$$

Boundary conditions:

$$T(x, t) = \mu(x, t) \quad x \in \Gamma \equiv \partial\Omega, t > 0$$

Numerical treatment of the problem

$$M \frac{dT}{dt} + KT = F$$

Note: $f(x, t, T)$ connects the system with heat sources in the food camera. The heat is supplied to the source material by radiation, conduction or combination of both types.

Mass matrix:

$$M = \left[\int_{\Omega} c \rho \phi_i \phi_j \, dx \right]_{i,j=1}^N$$

Stiffness matrix:

$$K = \left[\int_{\Omega} k \nabla \phi_i \nabla \phi_j \, dx \right]_{i,j=1}^N$$

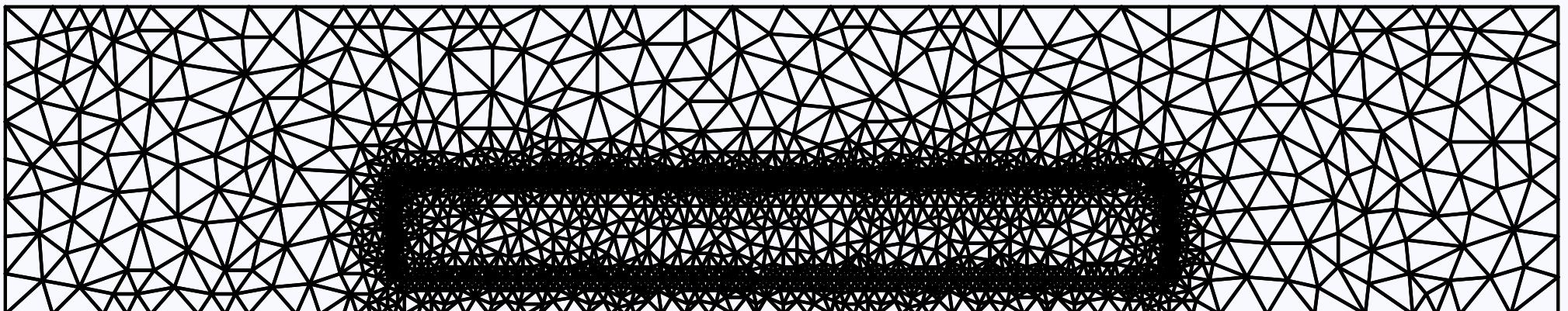
Right hand side:

$$F = \left[\int_{\Omega} f(x, t, T) \phi_i \, dx \right]_{i=1}^N$$

The coarser finite element mesh

Number of nodes: 6568

Number of elements: 12819



Solving the systems of linear equations

After the variational formulation, the problem is discretized by the linear triangular finite elements in space (minimal angle of a triangle, maximal area of a single triangle) and the simplest finite differences in time. For the uniform discretization of the time interval ($t_j = t_0 + j \tau$, where τ is the time stepsize), we get the following simple algorithm:

for $j = 1, \dots, N$:

compute $b = (M - \tau(1-\vartheta)K)T^{j-1} + \tau\vartheta F^j + \tau(1-\vartheta)F^{j-1}$

find T^j : $(M + \tau\vartheta K)T^j = b$

end for

We restrict our attention to implicit methods with $\vartheta \in \langle \frac{1}{2}, 1 \rangle$. Particularly, we shall consider two cases with $\vartheta = \frac{1}{2}$ and $\vartheta = 1$, which correspond to Crank-Nicholson (CN) and backward Euler (BE) method, respectively.

Adaptive time steps

The time interval is divided by time steps $t_0 < t_1 < \dots < t_{N-1} < t_N$ and $\tau_j = t_j - t_{j-1}$.

for $k = 1, 2, \dots$ until *stop*:

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find  $T^{k+1}$ :  $(M + \tau^k K) T^k = M T^{k-1} + \tau^k F^k$  // for the BE steps is  $\vartheta = 1$ 
compute  $r = (M + \frac{1}{2}\tau^k K) T^k - (M - \frac{1}{2}\tau^k K) T^{k-1} - \frac{1}{2}\tau^k F^k - \frac{1}{2}\tau^k F^{k-1}$ 
compute  $\eta^k = \|r\|/\|T^k\|$  // we suppose  $T_{CN} \simeq T_{BE} - r$ 
decide if  $\eta^k < \varepsilon_{\min}$  then  $\tau^{k+1} = 2\tau^k$  // in usual practice, we specify
      if  $\eta^k > \varepsilon_{\max}$  then  $\tau^{k+1} = \tau^k/2$  //  $\varepsilon_{\min} = 10^{-8}$ ,  $\varepsilon_{\max} = 10^{-7}$ 
      if  $\eta^k \in (\varepsilon_{\min}, \varepsilon_{\max})$  or  $(\eta^k < \varepsilon_{\min} \text{ and } \eta^{k-1} > \varepsilon_{\max})$  then
           $\tau^{k+1} = \tau^k$  and  $T^{k+1} = T^k$ , stop
      if  $\eta^k > \varepsilon_{\max}$  and  $\eta^{k-1} < \varepsilon_{\min}$  then
           $\tau^{k+1} = \tau^k/2$  and  $T^{k+1} = T^{k-1}$ , stop
end for
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How often to perform the ATS procedure ?

The adaptivity test depends on the input parameters ε_{\min} , ε_{\max} and is performed each $\#N_{NA}$ time steps. The time interval is 5000 s and the adaptive time stepping begins with $\tau = 5$.

The linear system is solved up to the relative residual accuracy 10^{-9} . The *exact* solution vector T_{ex} means the solution of the linear system for the constant time stepsizes (no adaptivite time steps, $\tau = 5$, Time = 109.07 s, #It = 33067, $\#N_{TS} = 999$).

ε_{\min}	ε_{\max}	$\#N_{NA}$	Time [s]	#It	#It _A	$\#N_{TS}$	τ_*	$\frac{\ T - T_{ex}\ _2}{\ T\ _2}$	$\ T - T_{ex}\ _\infty$
10^{-8}	10^{-7}	0	28.47	8515	8515	104	48.1	$3.87 \cdot 10^{-6}$	$1.53 \cdot 10^{-3}$
10^{-8}	10^{-7}	2	20.40	6700	3110	88	56.8	$4.68 \cdot 10^{-6}$	$1.88 \cdot 10^{-3}$
10^{-8}	10^{-7}	4	15.89	5540	1513	77	64.9	$3.31 \cdot 10^{-6}$	$1.36 \cdot 10^{-3}$
10^{-8}	10^{-7}	8	18.19	6225	1204	95	52.6	$5.55 \cdot 10^{-6}$	$2.32 \cdot 10^{-3}$
10^{-8}	10^{-7}	16	17.66	6073	664	99	50.5	$5.55 \cdot 10^{-6}$	$2.32 \cdot 10^{-3}$
10^{-8}	10^{-7}	32	16.37	5661	366	93	53.8	$4.35 \cdot 10^{-6}$	$1.80 \cdot 10^{-3}$

ScLion: Pentium 4 / 1.5 GHz 256 L2 cache, 256 RAM, Scientific Linux 4.5, GNU C++ 4.1.1

How to set the parameters ε_{\min} , ε_{\max} ?

No adaptivite time steps, $\tau = 5$: Time = 109.07 s, #It = 33 067, #N_{TS} = 999).

ε_{\min}	ε_{\max}	#N _{NA}	Time [s]	#It	#It _A	#N _{TS}	τ_*	$\frac{\ T - T_{\text{ex}}\ _2}{\ T\ _2}$	$\ T - T_{\text{ex}}\ _\infty$
10^{-9}	10^{-8}	4	38.33	11869	2996	265	19	$2.17 \cdot 10^{-6}$	$8.18 \cdot 10^{-4}$
10^{-8}	10^{-7}	4	15.89	5540	1513	77	65	$3.31 \cdot 10^{-6}$	$1.36 \cdot 10^{-3}$
10^{-7}	10^{-6}	4	9.27	3321	929	37	135	$8.66 \cdot 10^{-6}$	$4.08 \cdot 10^{-3}$
10^{-6}	10^{-5}	4	3.71	1291	699	7	714	$2.86 \cdot 10^{-5}$	$2.29 \cdot 10^{-2}$
10^{-5}	10^{-4}	4	3.02	988	983	1	5000	$2.90 \cdot 10^{-5}$	$2.06 \cdot 10^{-2}$

Impact for the practical usage

For the given ε_{\min} , ε_{\max} : #N_{NA} $\in \langle 3, 15 \rangle$ with the preference of smaller values.

For the given ε_{PCG} : $\varepsilon_{\min} \in \langle \varepsilon_{\text{PCG}}, \varepsilon_{\text{PCG}} \cdot 10^2 \rangle$ and then $\varepsilon_{\max} = \varepsilon_{\min} \cdot 10$.

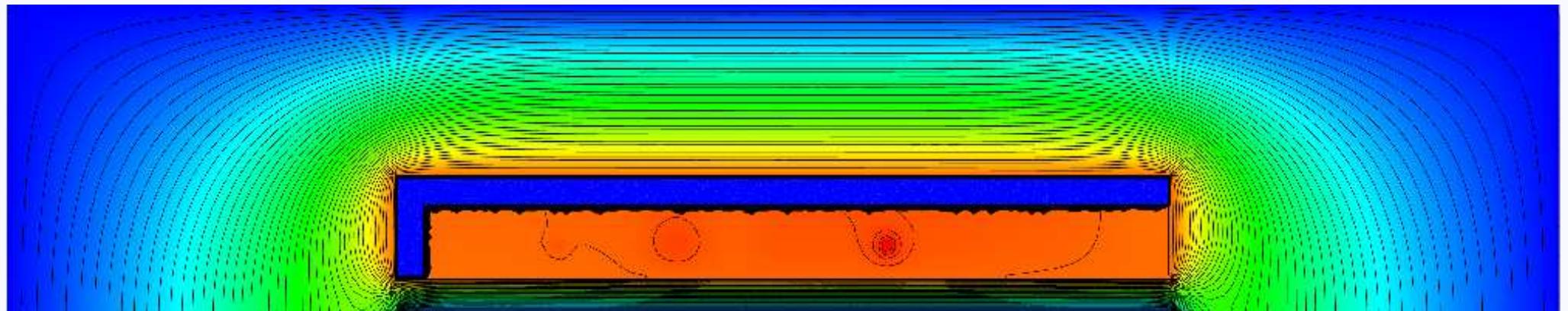
Numerical experiments in the full time interval

The considered time interval is set to be $760\,405\text{ s} \sim 8\text{ days } 19\text{ hours } 13\text{ minutes}$.

No adaptivite time steps, $\tau = 5$: Time = 16882.6 s, #It = 5 023 738, #N_{TS} = 152 082).

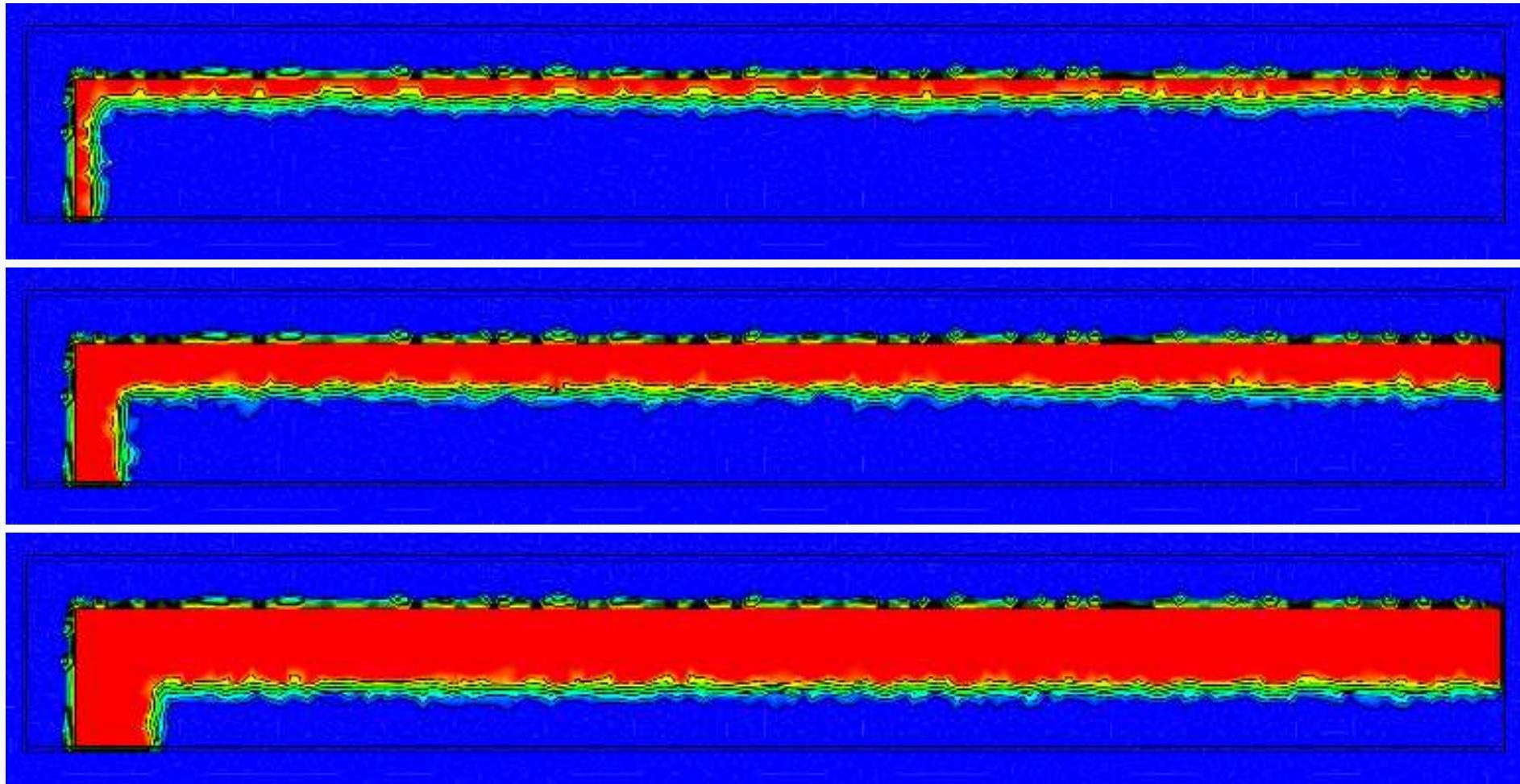
ε_{\min}	ε_{\max}	#N _{NA}	Time [s]	#It	#N _{TS}	τ_*	$\frac{\ T - T_{\text{ex}}\ _2}{\ T\ _2}$	$\ T - T_{\text{ex}}\ _\infty$
10^{-9}	10^{-8}	4	5539.4	1 711 902	35 880	21	$1.86 \cdot 10^{-6}$	$4.13 \cdot 10^{-4}$
10^{-8}	10^{-7}	4	2274.6	786 912	10 358	73	$6.09 \cdot 10^{-5}$	$1.85 \cdot 10^{-2}$
10^{-7}	10^{-6}	4	800.6	300 058	2 943	258	$1.19 \cdot 10^{-4}$	$2.29 \cdot 10^{-2}$

The temperature field at the end of time interval



From the engineering point of view

The water filling of the zeolites at the 1/3, 2/3 and 3/3 of the time interval.



Red: 100 % Yellow: 75 % Green: 50 % Cyan: 25 % Blue: 0 %

Conclusion

The introduced work is devoted to mathematical modelling of the freeze-drying process under high vacuum. Especially, it concerns the computer simulation of heat and mass transfer in the absorbent camera. The origin of such simulation is in solving the time-dependent nonlinear partial differential equation of parabolic type and the core is the repeated solution of linear systems for different time steps.

The existing program code used only the uniform discretization of the considered time interval, when the time stepsizes are constant. In an effort to optimize the whole simulation, we included the adaptive time stepping procedure in the code. This procedure is based on the local comparison of Crank-Nicholson and backward Euler time steps.

Finally, we performed the numerical experiments to know the behaviour of the resulting program, to find the optimal (in some sense) parameters and to try it on a selected real-life problem. The tests confirmed its big usefulness for practice.

Thank you for your attention