



Preventing the waste of animal source foods by predicting the kinetics of oxidation reactions

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Preventing the waste of animal source foods by predicting the kinetics of oxidation reactions

Reaction-diffusion modelling of a 44-reactions chemical scheme.

Jason Sicard, Alain Kondjoyan

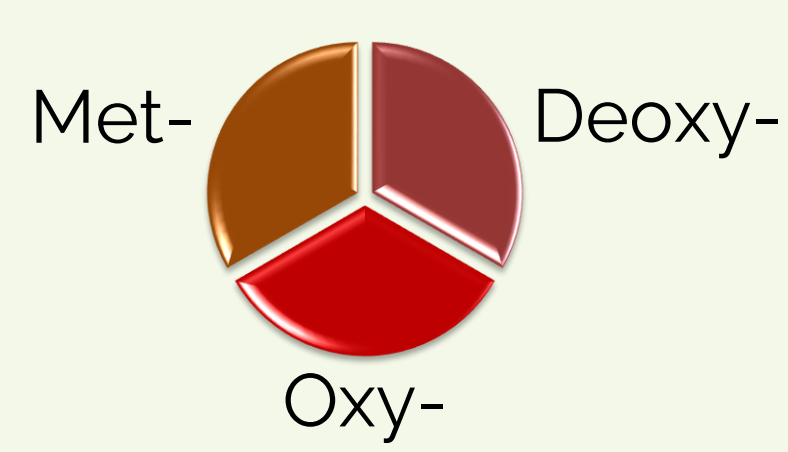
BACKGROUND



Carbon footprint
of meat



Consumers reject
brown-colour meat



Met- Oxy- Deoxy-
Myoglobin
influences colour



Modified Atmosphere
Packaging

OBJECTIVE



PREVISION OF
MYOGLOBIN
CHEMICAL STATE

MATERIAL AND METHOD

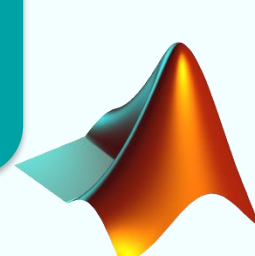
3 groups of reactions

❖ Myoglobin oxidation
reactions

O₂ ❖ mitochondrial respiration
❖ production of hydrogen
peroxide by glycolysis

Fe ❖ Fenton reactions
(non-heme iron)

Ao ❖ Water-soluble
antioxidants reactions



resolution of **diffusion** (finite-difference)
and **reactions** (ordinary differential equations)

$$\frac{d[C_i]}{dt} = \sum_{j=1}^N a_{ij} k_j \left(\prod_{i \in [1, M], a_{ij} < 0} [C_i]^{-a_{ij}} \right)$$



Rate constants literature

Sensitivity analysis
(homogeneous O₂)

• Simplified
reaction
scheme

Diffusion of O₂

• Reaction-
diffusion model

Optimization

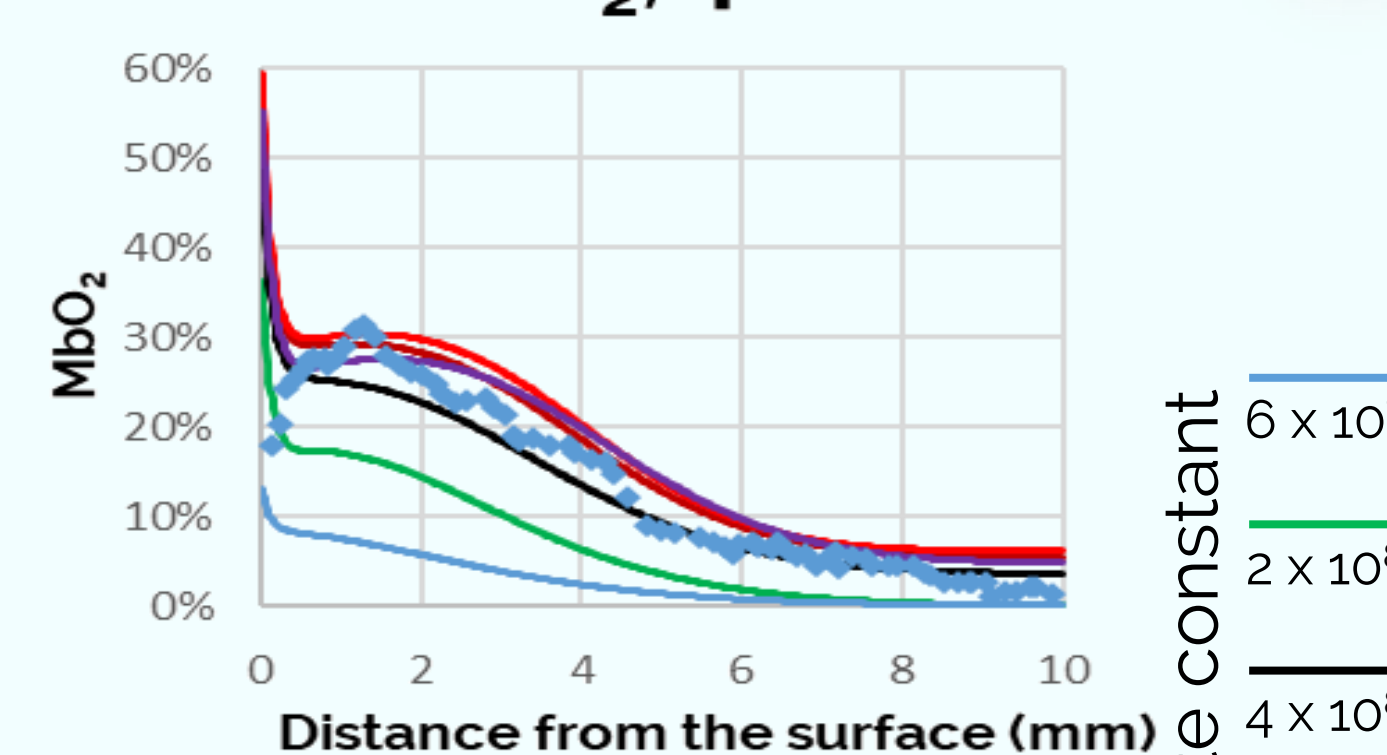
• Consolidated
rate-constant
values



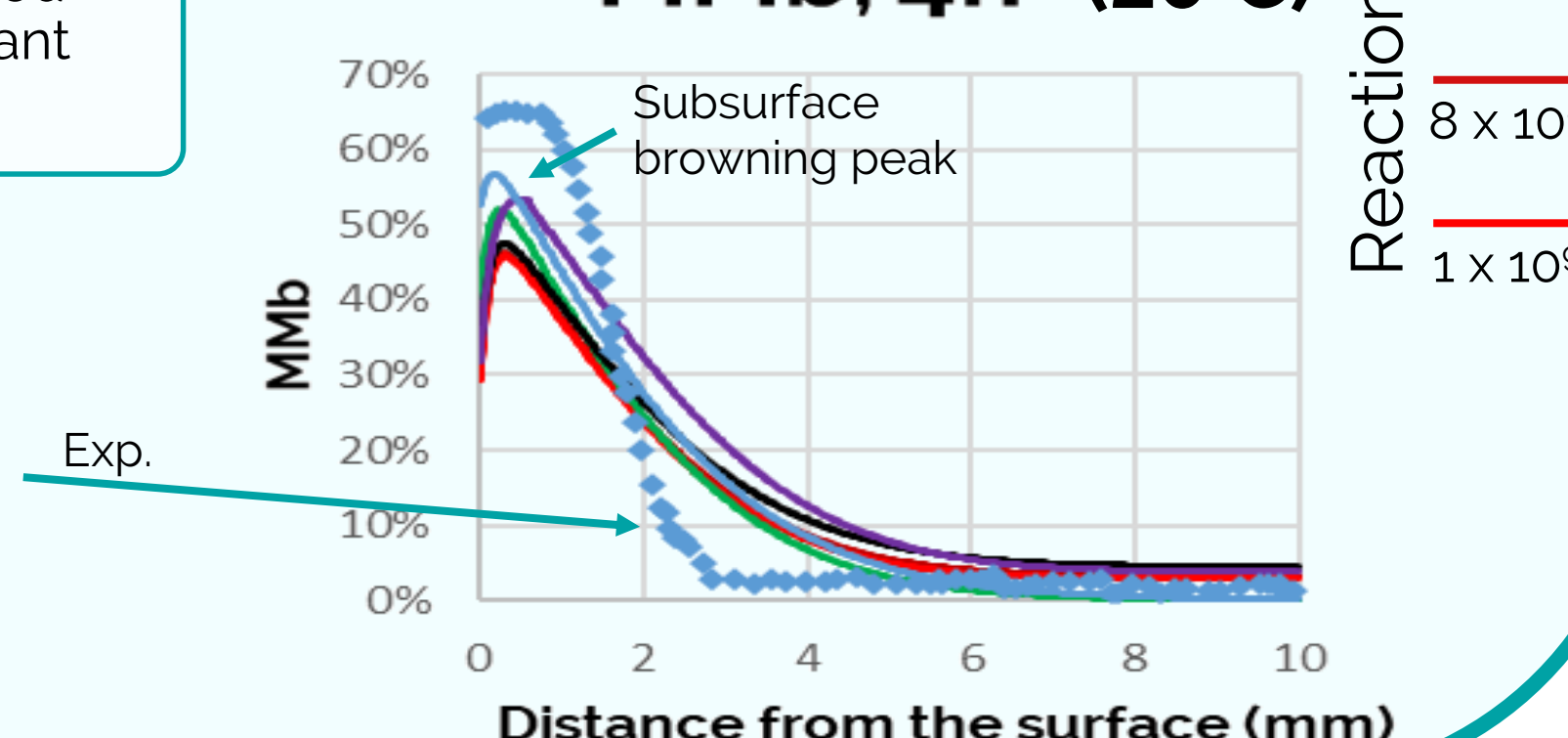
Validation with experimental
in-depth myoglobin profiles on
longissimus lumborum muscle

Ex. impact of the rate constant of the
oxidation of deoxymyoglobin reaction
 $MbFe^{2+} + O_2 \rightarrow MbFe^{2+}O_2$

MbO₂, 4h (20°C)

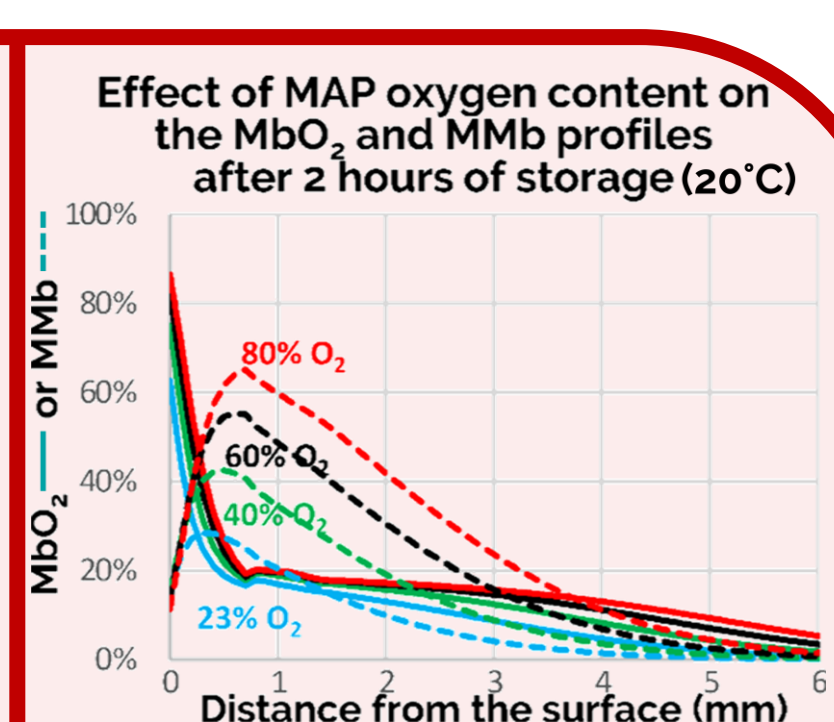


MMb, 4h (20°C)



RESULTS

- ❖ Water-soluble antioxidants offset the effect of Fenton chemistry on the shape of MbO₂ and MMb profiles.
- ❖ MAP extends the shelf-life of meat by increasing both CO₂ and O₂ to preserve the bright red colour. However, high oxygen also increases both the intensity and width of subsurface browning, eventually leading to a bright red surface covering a thick brown meat.



22 reactions
optimized*
scheme

*to provide the same results as the complete scheme for the targeted compounds (myoglobin states, oxygen and hydrogen peroxide)

DISCUSSION

- ❖ This model allows for the identification of conditions leading to colour instability or other phenomena sometimes observed in practice when using MAP.
- ❖ The influence of a change in environmental conditions on microorganisms and microorganisms' influence on colour and safety also need to be considered.
- ❖ Supplemental comparison data is needed to evaluate the activation energy of reactions. (see 2nd ref.)
- ❖ Multi-compartments modelling would be required to go further, notably to account for marbling fat particles and the reactions that take place in them.
- ❖ This methodological approach successfully represented a complex scheme of reactions involved in the variation of surface quality of a solid food and is **applicable to other foods!**



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References:

Kondjoyan, A.; Sicard, J.; Badaroux, M.; Gatellier, P. Kinetics Analysis of the Reactions Responsible for Myoglobin Chemical State in Meat Using an Advanced Reaction-Diffusion Model. *Meat Science* **2022**, *191*, 108866, doi:[10.1016/j.meatsci.2022.108866](https://doi.org/10.1016/j.meatsci.2022.108866).

Kondjoyan, A.; Sicard, J.; Cucci, P.; Audonnet, F.; Elhayel, H.; Lebert, A.; Scislawski, V. Predicting the Oxidative Degradation of Raw Beef Meat during Cold Storage Using Numerical Simulations and Sensors—Prospects for Meat and Fish Foods. *Foods* **2022**, *11*, 1139, doi:[10.3390/foods11081139](https://doi.org/10.3390/foods11081139).