



Multi-response modeling of acrylamide formation in biscuits

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Background

During baking of biscuits potentially harmful compounds might form such as acrylamide (ACR). Kinetic modelling of ACR is a valuable tool for obtaining insight into the mechanism of its formation. Multi-response modelling, i.e. a modelling approach based on the fundamental chemical reaction pathways, has the advantage of improving the precision of kinetic parameters estimates while providing insight on the actual reaction mechanism.

Objective

The aim of this study was to model acrylamide formation during baking of biscuits, using multi-response kinetic modelling.

Materials and methods

A biscuit formulation (table 1) was baked in a conventional oven at 200 °C for different times. Concentrations of ACR as well as of sucrose, glucose, fructose, total free amino acids (AA), and asparagine were measured in the samples along with moisture content and temperature. Multi-response modelling was performed using the Athena Visual Studio software package (Athena Visual Software Inc., Naperville, IL, USA).

Table 1. Composition of the biscuit recipe.

Ingredient	Amount (g)
Wheat flour (standard T55/W150 flour)	80
Refined palm oil	20
Sucrose	35
NaCl	1
Water	17.6
Sodium bicarbonate	0.8
Ammonium bicarbonate	0.4

Results

Several kinetic schemes were formulated and applied to the entire baking time range (0-15 minutes). During baking, sucrose hydrolysis and reducing sugars formation were limited up to 11 minutes after which a constant increase in sucrose hydrolysis rate occurs. This behaviour could not be accounted for solely by a kinetic reaction scheme. Only 4 time points (12-15 minutes) were thus considered for further modelling. The changes in moisture content and temperature (<5°C) were negligible in the selected time range. The model that produced the best fit to the experimental data was selected by a model discrimination analysis based on the posterior probability criterion (figure 1 and 2). In table 2 the optimal estimates for the kinetic parameters is reported.

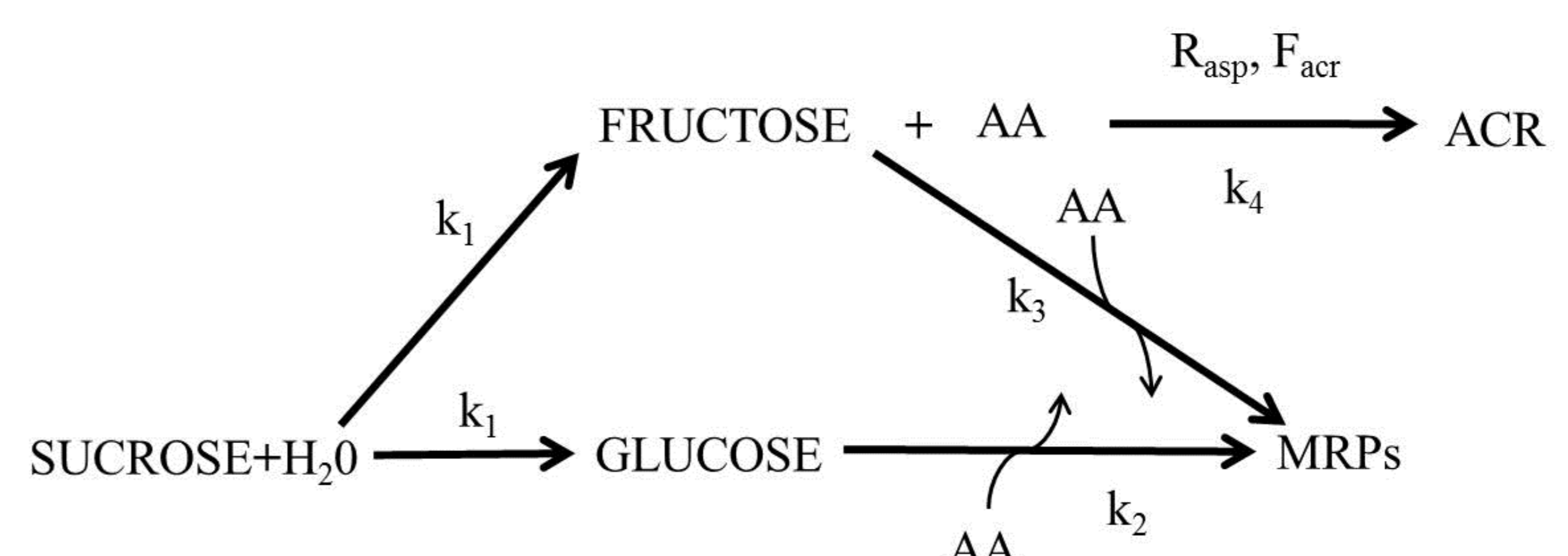


Figure 1. Simplified kinetic scheme selected by model discrimination analysis. MRPs=Maillard reaction products.

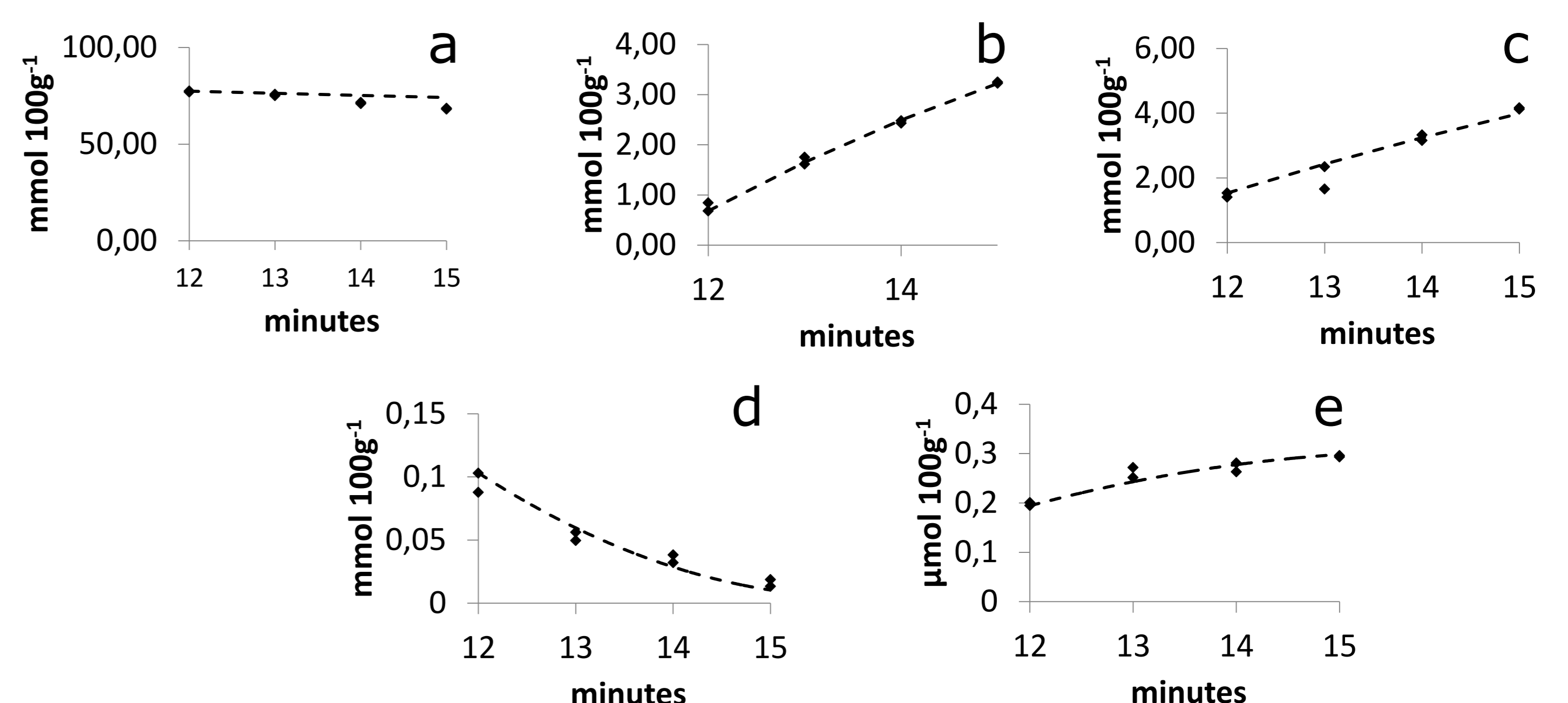


Figure 2. Fit of the predicted values to the experimental data for: a) sucrose, b) glucose, c) fructose, d) total amino acids, e) acrylamide.

Only fructose contributes to ACR formation. The fraction of asparagine to total AA (R_{asp}) was approximately constant during baking and the fraction of asparagine converted to ACR (F_{acr}) is included in the model as a parameter. AA are only degraded upon reaction with fructose whereas the contribution of intermediate carbonyls from Maillard reaction is negligible. The fit was good for reducing sugars, total AA and ACR whereas the extent of sucrose hydrolysis was partially underestimated.

Table 2. Parameters estimate for the selected kinetic model.

Parameter	units	Optimal estimate ($\times 10^2$)	95% confidence interval ($\times 10^2$)
k_1	$\text{mmol}^{-1} 100\text{g s}^{-1}$	1.45	± 0.23
k_2	s^{-1}	12.4	± 8.90
k_3	s^{-1}	8.86	± 7.58
k_4	s^{-1}	27	± 5.3
F_{acr}		0.74	± 0.094

Conclusions

A simplified multi-response kinetic model for ACR formation in biscuits baked is proposed which accurately predicts ACR evolution during baking at 200 °C in the range 12-15 minutes. For its application to the entire time range, additional physical and chemical information beside the chemical reaction network must be incorporated in the model.

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