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Virtual occlusal definition for orthognathic surgery

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Abstract. Computer-assisted surgical simulation is being used increasingly in orthognathic surgery. However, occlusal definition is still undertaken using model surgery with subsequent digitization via surface scanning or cone beam computed tomography. A software tool has been developed and a workflow set up in order to achieve a virtual occlusal definition. The results of a validation study carried out on 60 models of normal occlusion are presented. Inter- and intra-user correlation tests were used to investigate the reproducibility of the manual setting point procedure. The errors between the virtually set positions (test) and the digitized manually set positions (gold standard) were compared. The consistency in virtual set positions performed by three individual users was investigated by one way analysis of variance test. Inter- and intra-observer correlation coefficients for manual setting points were all greater than 0.95. Overall, the median error between the test and the gold standard positions was 1.06 mm. Errors did not differ among teeth (F = 0.371, P > 0.05). The errors were not significantly different from 1 mm (P > 0.05). There were no significant differences in the errors made by the three independent users (P > 0.05). In conclusion, this workflow for virtual occlusal definition was found to be reliable and accurate.

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Virtual simulation, based on three-dimensional (3D) image planning systems, is used increasingly for preoperative planning of orthognathic surgery.^{1–6} Commercially available software packages provide convenient tools for 3D measurements, virtual osteotomy, bone segment repositioning, and soft tissue prediction. However, few of the currently available software packages provide tools for virtual occlusal definition.

In the current computer-assisted surgical simulation (CASS) workflow, the final occlusion is decided manually using model surgery with subsequent digitization via surface scanning procedures or cone beam computed tomography (CBCT).^{7–9} As well as being time-consuming and often inaccurate, the main drawback of this model surgery based-approach is that it cannot fully enable the surgeon to visualize how the final occlusion may change the morphology of the surrounding hard and soft tissues in 3D.¹⁰

A software tool has been developed and a workflow set up in order to achieve a virtual occlusal definition within the present CASS protocol. A validation study was carried out to test its accuracy and reliability.

Materials and methods

This study was performed at a university school and hospital of stomatology in Beijing, China. The research protocol was approved by the institutional ethics committee.

Workflow of the virtual occlusal definition

The software tool was developed to realize a virtual occlusal definition based on visualization support and precise movements. A virtual workflow was set up accordingly.



Fig. 1. Manual marking of the marker points. A total of 37 pairs of corresponding marker points are identified manually using a feature point-marking interface. These are the cusp and fossa points on each tooth.

First, the digital model data of the upper and lower jaws are imported into the virtual system. Thirty-seven pairs of corresponding marker points are then identified manually (Fig. 1). Vectors are generated automatically between the upper points and the corresponding lower points, based on the principles of prosthodontics and orthodontics. For example, the mesiobuccal cusp point on the maxillary first molar is aligned with the buccal fissure point of the opposing mandibular first molar. The length and direction of vectors are determined by the distance and direction between theoretical corresponding points in the upper and lower jaws.

Second, with the lower dentition set as a fixed object, the position of the upper jaw is adjusted using an interactive adjustment tool, so as to align it with the lower jaw. Users are able to move the upper dentition

either by typing in instructions in a dialog box (Fig. 2A) or by using a free-hand module (Fig. 2B). Rotation and transposition along a single axis makes movement easier to handle than with 3D adjustments. During the adjustment, two representative tools assist users to obtain information about the relationship between the cusp– fossa and tooth contact.

The collision heat map tool shows the vertical distance and contact between corresponding points using a colour scale. A collision detection algorithm calculates whether points on the upper and lower dentitions are in contact with, or overlap each other (Fig. 2C). Contact detection is only looked for in a small region, near the occlusal plane. This greatly reduces the calculations required, helping the software run smoothly.

The distance projection tool shows the directions of occlusal deviations. Vectors between corresponding points are projected onto the occlusal plane to determine sagittal and transverse deviations (Fig. 2D). In an ideal occlusion, bilateral vectors should be symmetrical in direction and length. Users



Fig. 2. Software tool for virtual occlusal definition. (A) Motivation dialog box: the user can adjust the position of the upper dentition by typing parameters into the box. (B) Free-hand engine: the user can move or rotate the upper dentition along a single direction by dragging the axis or circles freely using the mouse. (C) Collision heat map: the vertical distances between the upper and the lower dentitions are shown on a colour map. (D) Distance projection view: vectors between corresponding points are projected onto the occlusal plane to demonstrate sagittal and transverse deviations. (E) Adjustment hint grid view: this includes seven single-direction automatic minor revision tools that are applied when the upper and lower dentitions are close to each other. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

can make adjustments by following these vectors.

Third, when the upper and lower jaws are near to final occlusion, adjustment tools in 'adjustment hint grid view' (Fig. 2E) are used to make automatic minor regulations. There are seven types of single-direction movement in the hint grid, including transverse transposition, rotation, sagittal transposition, and coronal rotation of the upper and lower jaws. The movements are calculated automatically, in real-time, according to parameters for a normal overjet, overbite, and better symmetry of bilateral vectors.

Every adjustment is aligned automatically and in real-time with every view on the interface. The user can revise the position of the upper jaw through an adjustment– gaining knowledge–further adjustment operation cycle until an optimal occlusion relationship is obtained. The workflow diagram is shown in Fig. 3.

Validation tests

The validation tests were designed to address three points: (1) Whether the manual procedure of identifying marker points has good inter- and intra-observer reproducibility. (2) Whether the present workflow is accurate. (3) Whether the result of virtual occlusal definition by different users is consistent.

Therefore, three tests were performed: a reproducibility test for the manual procedure for marking points (test 1), an accuracy test (test 2), and a reproducibility test (test 3) for virtual occlusal definition.

According to the sample size calculation, assuming a desired power of 0.95, type I error rate (α) of 0.05, and an effect size of 0.5, 60 volunteers (30 female and 30 male) were required for this study. The inclusion criteria were the following: (1) northern Han Chinese ethnicity; (2) age between 18 and 27 years; (3) class I incisor relationship with overjet and overbite between 1 and 4 mm; and (4) Angle class I molar relationship. The exclusion criteria were as follows: (1) previous tooth loss or restorations; (2) obvious tooth torsion and uneven tooth length; (3) a history of orthodontic treatment; (4) severe caries with complete destruction of the occlusal surface; (5) obvious dental crowding; and (5) periodontal problems, such as gingival recession or periodontitis.

Impressions of the upper and lower jaws were recorded using silicon impression materials (Silagum-Putty Light; DMG, Hamburg, Germany) and were subsequently poured with super hard plaster (Labstone; Heraeus, Hanau, Germany) to fabricate dental casts. Digital dental models of the upper and lower dentitions were obtained using a 3D photo-optical scanner (Smart Optics/Activity 102; Model-Tray GmbH, Hamburg, Germany) with a resolution of 0.1 mm. Data were saved in stereolithography (STL) format.

The relationship between the upper and lower plaster casts was identified manually by one prosthodontist, fixed using silicone resin (O-Bite; DMG), and then digitized using a double scanning protocol⁹ with the same 3D scanner. The position of the upper dentition was set as the gold standard. Thirty-seven pairs of corresponding marker points were identified manually by users on each tooth and all the

co-ordinate parameters were saved for reference (Fig. 4, upper row). The relationship between the upper and lower dentitions was then disturbed (Fig. 4, middle row) for purposes of the validation test. Users adjusted the upper jaw to achieve an optimized occlusion by following the virtual workflow (Fig. 4, lower row). When a user established an optimal occlusion, the position of the upper dentition was set as the test position. All the feature points were aligned with the upper jaw during the adjustment, so the difference between the gold standard and the test positions could be analyzed by the movement of feature points.

Statistical analysis

Errors were defined as the three-dimensional distance between the same feature point on the gold standard upper jaw (x_1) and the user-adjusted upper jaw (x_2) . This was measured as the distance between the original co-ordinate parameters (x_1, y_1, z_1) and the final co-ordinate parameters (x_2, y_2, z_2) of the same marker point. No superimposition was necessary. The distance between x_1 and x_2 was calculated using the equation:

$$D = \sqrt{(x_1 - x_2)^2 + (y_1 - y_2)^2 + (z_1 - z_2)^2}$$

. Given that there were multiple points on each tooth, the average error for each tooth was calculated as: $\Delta = \sum_{n=1}^{n} D/n$.

Test 1: Reproducibility test for the procedure of manually identifying marker points

Thirty of the 60 models were selected randomly for reproducibility testing. One investigator identified the marker points three times each on all 30 models, with a minimum interval of 24 h between markings. In addition, three individual investigators identified the marker points once on all 30 models. Inter- and intraobserver correlation coefficient tests were performed to check the reliability of the procedure.

Test 2: Accuracy test for the virtual occlusal definition

A single researcher established virtual occlusion in all 60 models. Descriptive statistics were used to investigate the error between the test and the gold standard positions. One-way analysis of variance (ANOVA) was performed to examine if the error was different between different teeth. An error of up to 1 mm was considered



Fig. 3. Workflow for virtual occlusion definition.



Fig. 4. Validation test for the accuracy of virtual occlusal definition. Upper row: Original relationship between the upper and lower dentitions. The colour heat map shows good contact and the vector projection view shows a symmetric corresponding relationship between the feature points. Middle row: The original relationship between the upper and lower dentitions is disturbed by moving the upper dentition. The visualization window shows an inappropriate correlation. The collision heat map is blue, indicating an increased vertical distance. The distance projection view shows markedly asymmetric vector distribution, indicating that the upper jaw is to the left of the lower jaw. Lower row: Virtual occlusal definition. The visualization window shows a normal relationship between each cusp and fossa. The collision heat map is green, indicating that the marker points are in contact with each other without colliding. The distance projection view shows bilateral symmetry in the length and direction of vectors. All illustrations for the virtual occlusal definition (lower row) are similar to those of the upper row. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

as the limit of tolerance for final occlusion. Errors above 1 mm were compared with *t*-tests.

Test 3: Reproducibility test for virtual occlusal definition by different users

Thirty of the 60 models were selected randomly for reproducibility testing. Three researchers independently established virtual occlusions in the 30 models. One-way ANOVA was performed to determine whether the positions set by different users were significantly different from each other.

For all the comparisons, P < 0.05 was considered statistically significant.

Results

In test 1, inter- and intra-observer correlation coefficients for the manual marking of marker points were all greater than 0.95, indicating the procedure to be highly reproducible among different users and different operations by one user.

In test 2, the median overall points error was 1.06 mm; the 90th and 95th percentile statistics were 1.70 mm and 2.00 mm, respectively. The median individual tooth errors varied from 0.94 mm to 1.10 mm. Details of errors between testing and gold standard positions are shown in Table 1.

Table 1. Errors between the test position and the gold standard for each tooth.

	Median (mm)	Perce	entiles
	Wedian (mm)	90th (mm)	95th (mm)
T17	1.10	1.96	2.30
T16	1.06	1.73	2.03
T15	1.05	1.48	1.93
T14	0.97	1.56	1.88
T13	1.00	1.78	1.95
T12	0.97	1.85	2.04
T11	1.00	1.81	2.07
T21	0.98	1.74	2.12
T22	0.99	1.67	2.20
T23	0.99	1.70	2.12
T24	0.94	1.66	1.90
T25	0.95	1.70	2.00
T26	0.94	1.74	2.23
T27	1.02	1.96	2.50
Overall	1.06	1.70	2.00

For each individual tooth, the error was not significantly greater than 1 mm (Table 2), and they did not differ significantly from each other (F = 0.371; P > 0.05) (Table 3). These results indicate that the position and the number of cusps and fossae do not affect the accuracy of occlusal definition.

In test 3, results showed that there were no significant differences between testing positions set by the three individual investigators for the *x*, *y*, and *z* axes (P > 0.05) (Table 4).

Discussion

Final occlusal definition is one of the key goals of preoperative design for orthognathic surgery. Compared to occlusal definition for dental prostheses, defining final occlusion for orthognathic surgery is more difficult. Attention must be paid not only to the stability, relationships between incisors and the first molar, and the overjet and overbite, but also to protrusion, symmetry, and facial contour.^{2,11,12} Therefore, a virtual tool of occlusal definition should provide users with comprehensive image illustrations and instructions for optimal occlusions.

Pongrácz and Bárdosi¹³ first reported a method for virtually defining occlusion by aligning upper and lower dental models on the basis of manually indicated corresponding points. The method focused on the corresponding relationships. Nadjmi et al.¹⁰ advanced the method by integrating a collision detection algorithm in the procedure and proved that the accuracy was approximately 1 mm, thus establishing a practical method for this purpose.

Building on these achievements, the present study aimed to improve the user-computer interaction and reasoning support, using the technique of visual analytics.¹⁴ The collision heat map and

Table 2. One-sample test between the error for each tooth and 1 mm.

	t A	đf	df <i>P</i> -value	Mean difference	95% CI of the difference	
	l	ui			Lower	Upper
T17	1.653	59	0.104	0.101	-0.021	0.223
T16	1.653	59	0.104	0.101	-0.021	0.223
T15	0.681	59	0.499	0.038	-0.074	0.149
T14	0.291	59	0.772	0.016	-0.092	0.123
T13	1.109	59	0.272	0.063	-0.051	0.178
T12	1.262	59	0.212	0.075	-0.044	0.194
T11	1.335	59	0.187	0.082	-0.041	0.204
T21	1.139	59	0.259	0.073	-0.055	0.202
T22	0.855	59	0.396	0.057	-0.077	0.192
T23	0.532	59	0.597	0.037	-0.102	0.177
T24	-0.033	59	0.974	-0.002	-0.136	0.132
T25	0.170	59	0.866	0.012	-0.129	0.153
T26	0.910	59	0.367	0.069	-0.082	0.220
T27	1.350	59	0.182	0.114	-0.055	0.282

CI, confidence interval.

the vector projection view were designed to enhance the illustration and reasoning support to users.

The collision heat map view aims to support the analysis of occlusal contact. In order to speed up the contact detection calculation, the algorithm was modified. Instead of 3D calculations, only contact perpendicular to the occlusal plane was calculated. By decreasing the computation time, users are provided with a real-time response whilst adjustments are being made. The vector projection view aims to support the analysis of corresponding relationships and stability. In the system, a theory-based algorithm is applied. Vectors are set up to visualize the relationship between the principle corresponding points, based on prosthodontic theory. Users obtain direct knowledge of occlusal deflection, overbite, and overjet from the direction and length of the vectors.

Instead of defining an initial corresponding relationship and then revising it, the present virtual tool serves users with a flexible interactive module during virtual occlusion establishment. The user can make adjustments and compromises among the different concerns, with visualization and reasoning support. This study should be regarded as a pilot, bringing the techniques of visual analytics into the specific medical setting of an interactive operation; the encouraging results should prompt further studies.

Nevertheless there are still weaknesses and limitations to the present study. An accuracy of 1 mm may be acceptable for orthognathic surgery planning,¹⁰ but it is not acceptable for some other applications, such as orthodontic-prosthodontic treatment. Further improvements in the virtual tool will be required. The principles of visual analytics imply that if a more theoretical computation is involved in reasoning, better results will be achieved. Therefore, the accuracy of the system presented here should be improved by integrating more medical specific information, such as the distribution of contact areas, occlusal force, and occlusal balance, in the visual analytic system.^{11,12,15}

The validation test was based on dentitions with normal occlusion, which were well established and stable. However, in patients with orthodontic decompensation, the occlusal relationship is often uncertain and unstable. Therefore, establishing occlusion is likely to be more difficult. For patients who have had segmental osteotomies, the technical requirements may be more demanding; collision detection on the lateral surfaces of the teeth and medical instructive information for dental arch matching may be needed. More validation

Table 3. Difference in the errors between different teeth.

	Sum of squares	df	Mean square	F	P-value
Between-group Within-group	1.260 216.006	13 826	0.097 0.262	0.371	0.979
Total	217.266	839			

Table 4. Reproducibility of the virtual occlusal definition for each axis among the three users.

	<i>x</i> -axis		y-axis		z-axis	
	F-value	P-value	F-value	P-value	F-value	P-value
T17	0.121	0.886	0.180	0.836	0.060	0.941
T16	0.076	0.927	0.262	0.770	0.057	0.945
T15	0.020	0.980	0.114	0.892	0.030	0.970
T14	0.011	0.989	0.109	0.897	0.026	0.975
T13	0.003	0.997	0.105	0.900	0.020	0.980
T12	0.001	0.999	0.119	0.888	0.015	0.985
T11	0.001	0.999	0.069	0.934	0.004	0.996
T21	0.001	0.999	0.066	0.937	0.003	0.997
T22	0.001	0.999	0.106	0.900	0.008	0.992
T23	0.003	0.997	0.084	0.919	0.010	0.990
T24	0.009	0.991	0.089	0.915	0.013	0.987
T25	0.019	0.981	0.111	0.895	0.016	0.984
T26	0.072	0.931	0.217	0.805	0.033	0.968
T27	0.117	0.890	0.145	0.865	0.037	0.964

tests are needed in further studies before the technique can be applied to real-life orthognathic cases.

The method presented for establishing virtual occlusion was found to be reliable and accurate.

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Competing interests

None.

Ethical approval

The research protocol was approved by the Institutional Ethics Committee of Peking University School and Hospital of Stomatology (No. IRB00001052-08048).

Patient consent

Not required.

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